EL891923376US

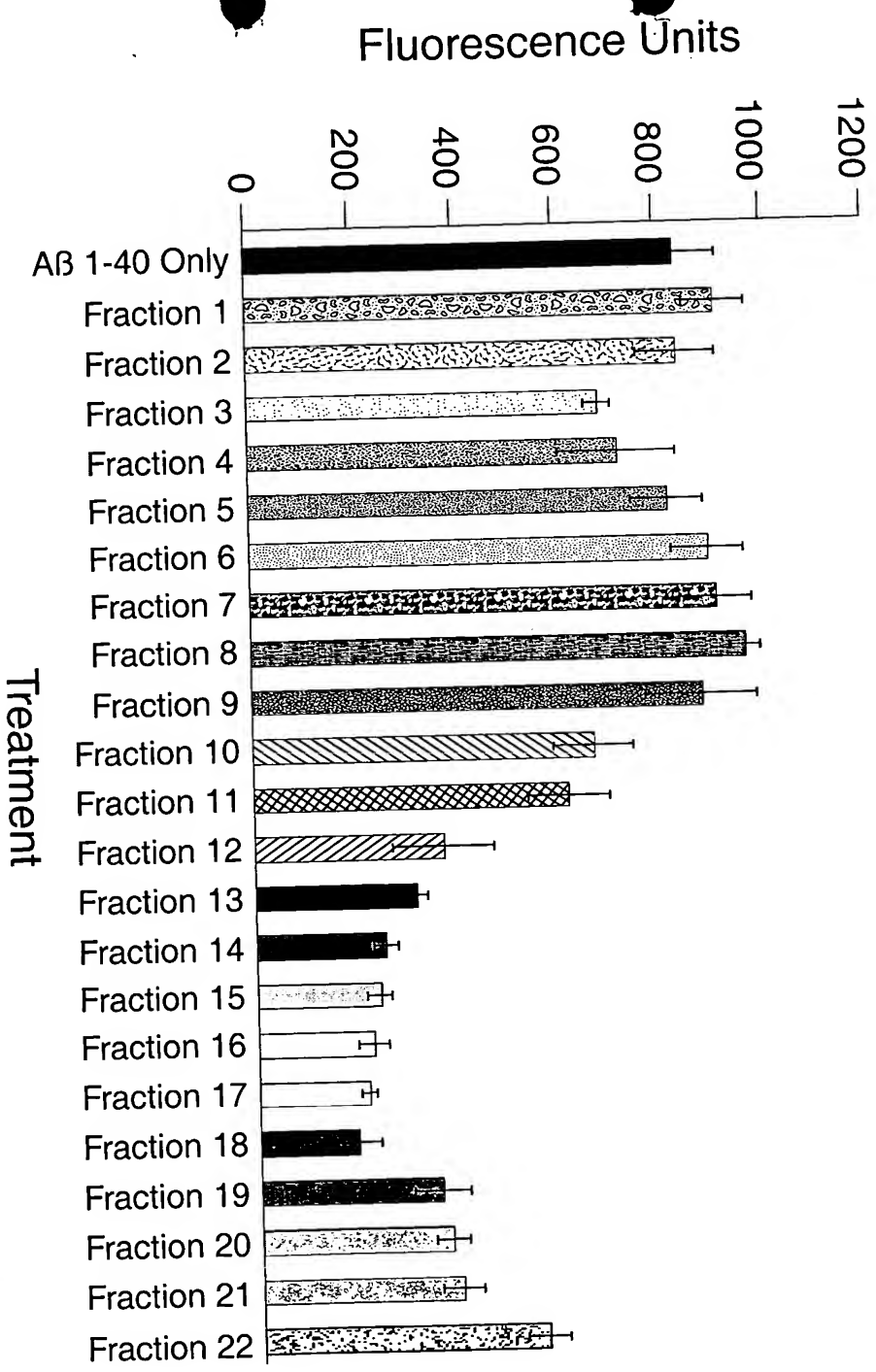


FIGURE 1

10053625.110201

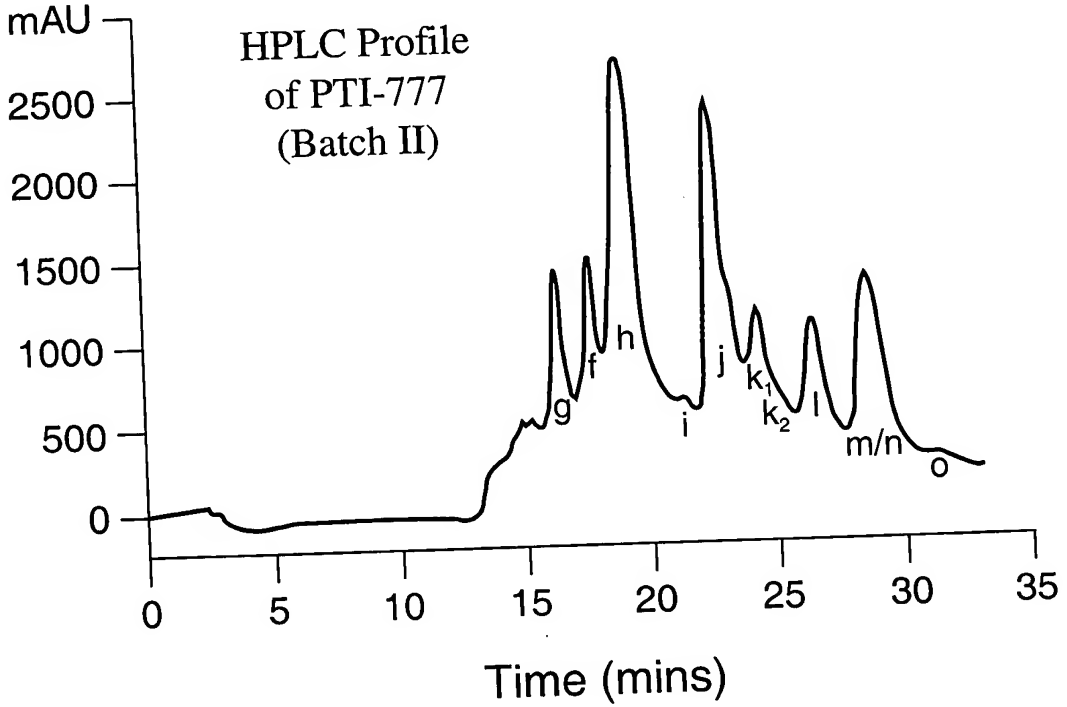


FIGURE 2

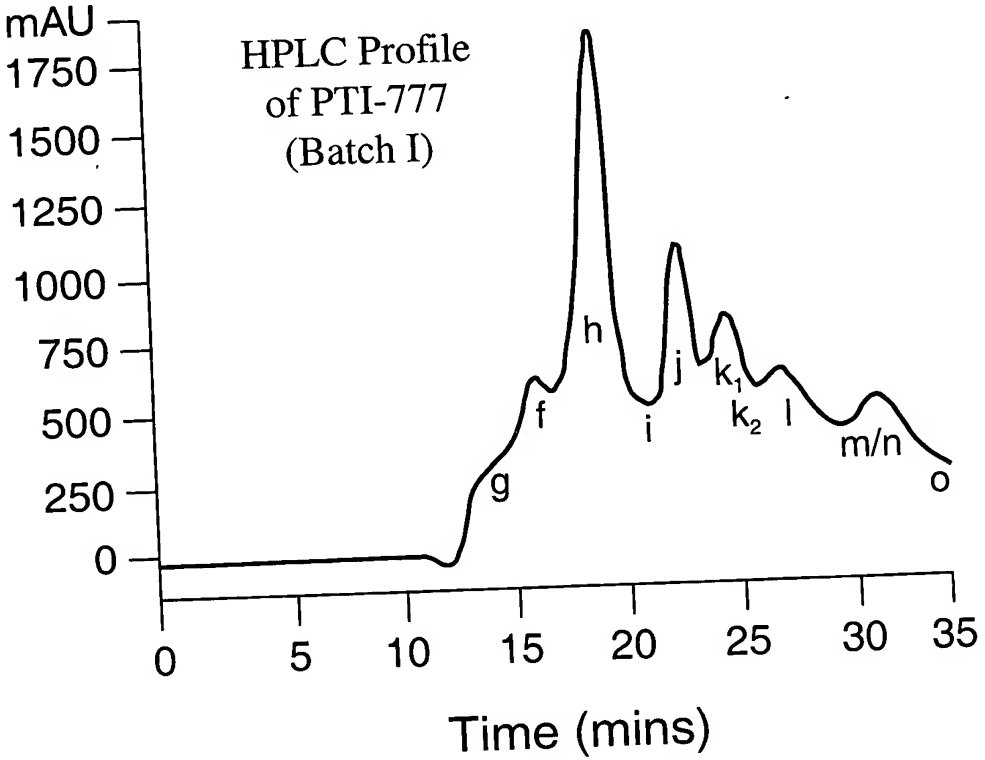


FIGURE 3

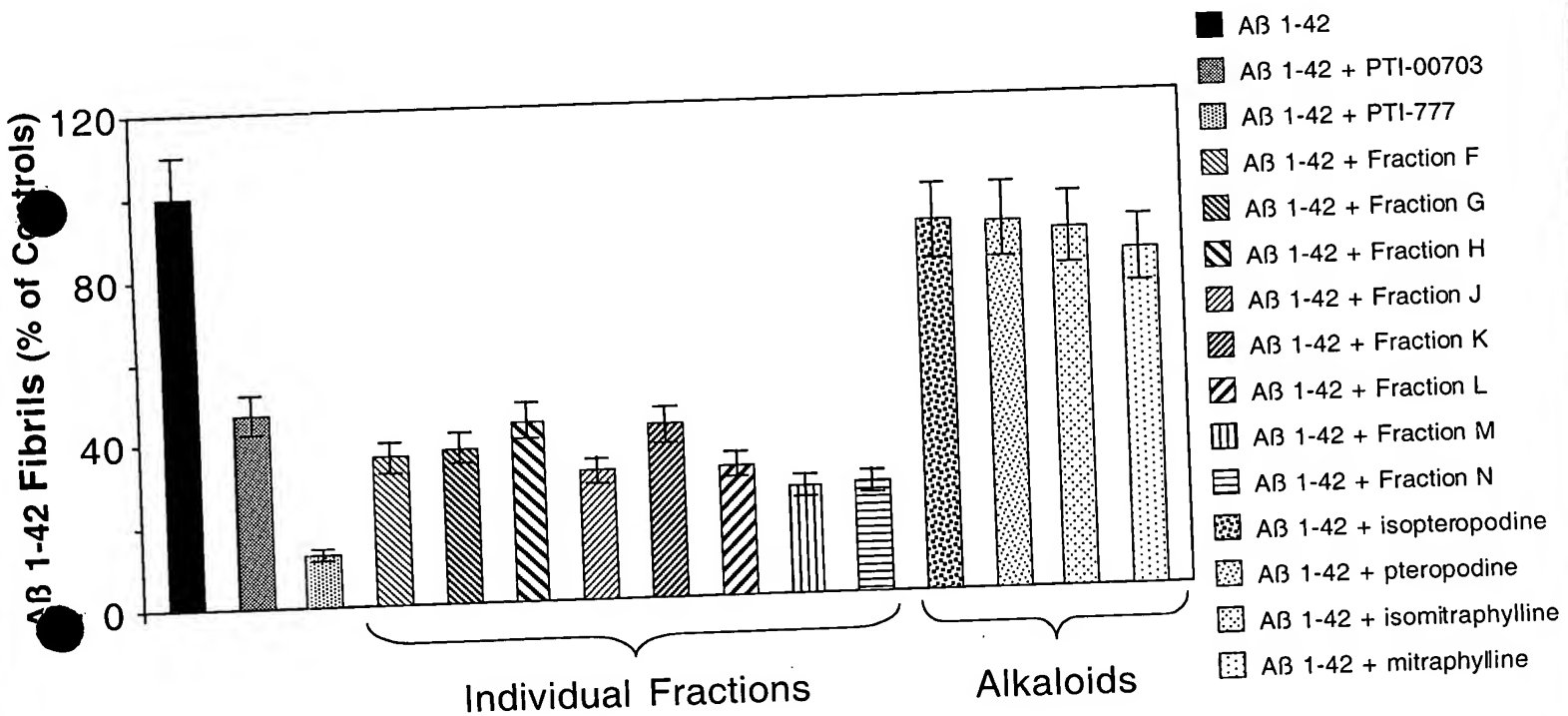


FIGURE 4

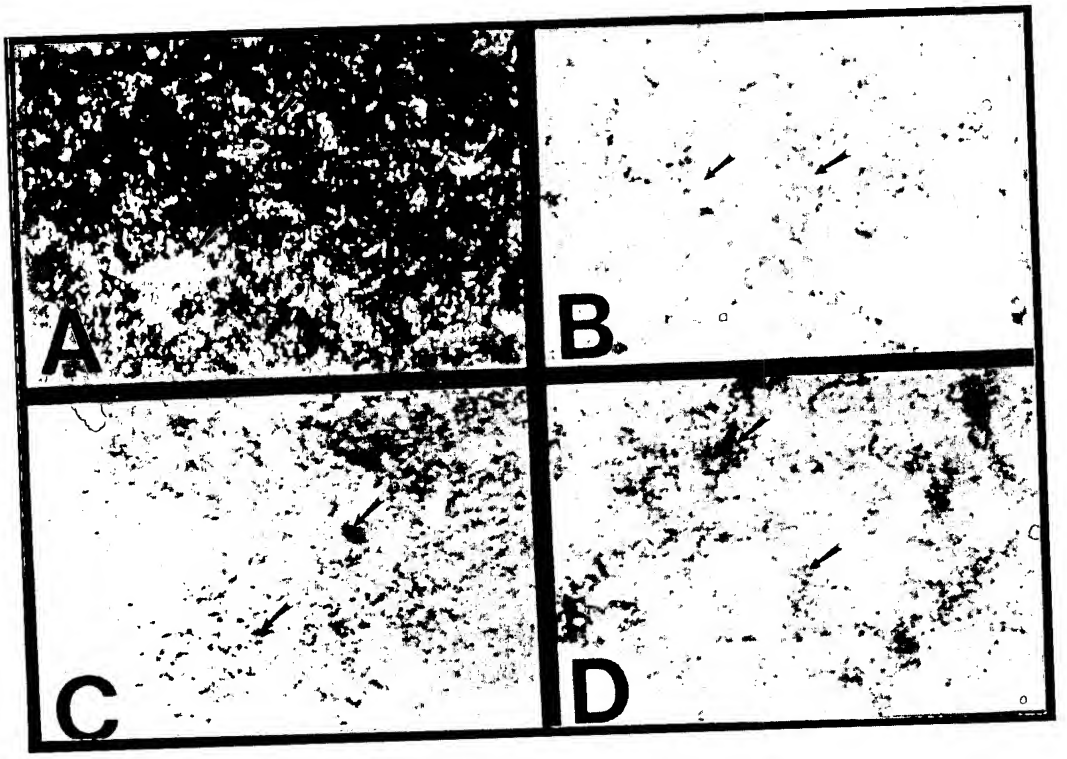


FIGURE 5

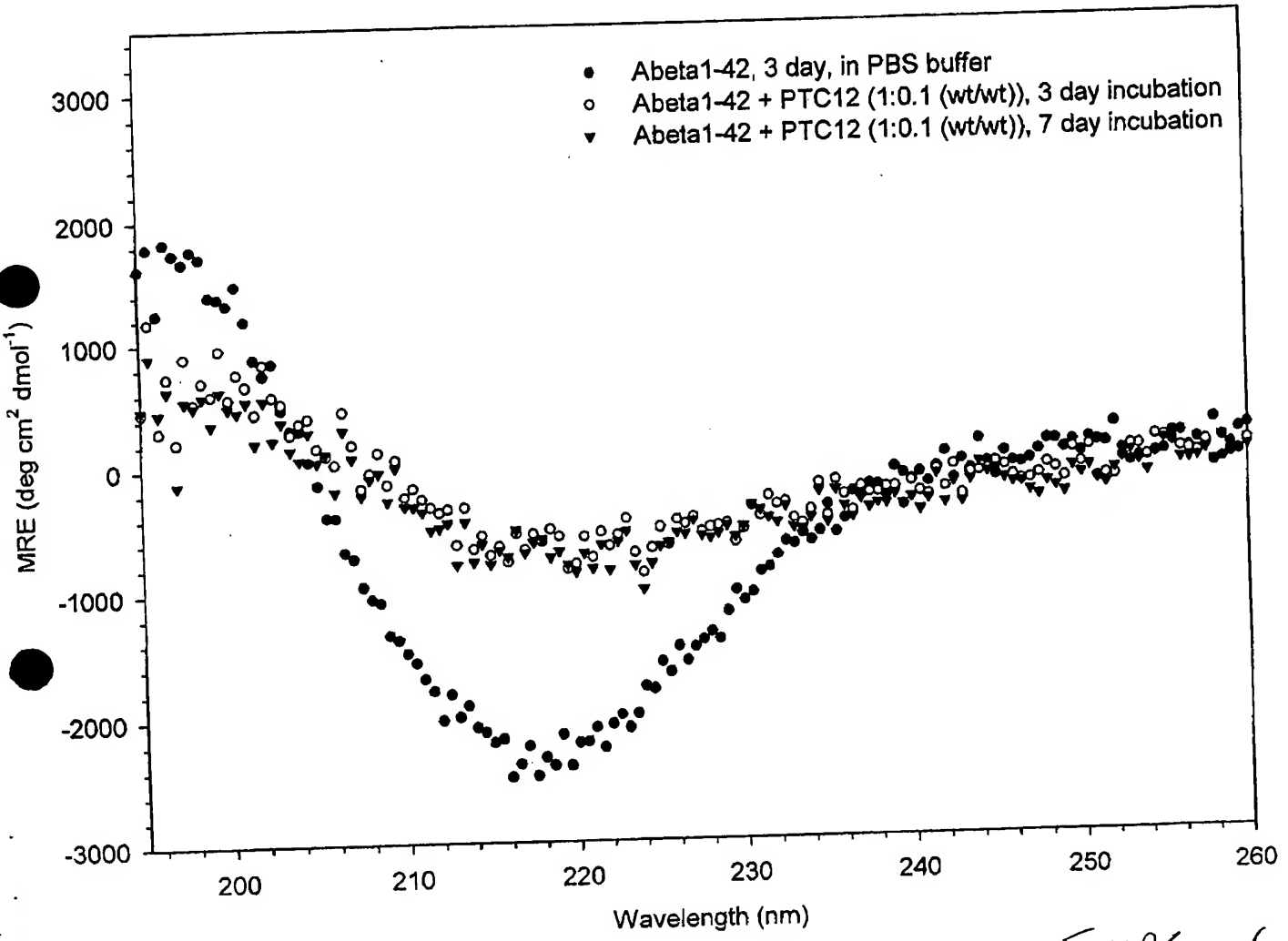


FIGURE 6

FIGURE 7

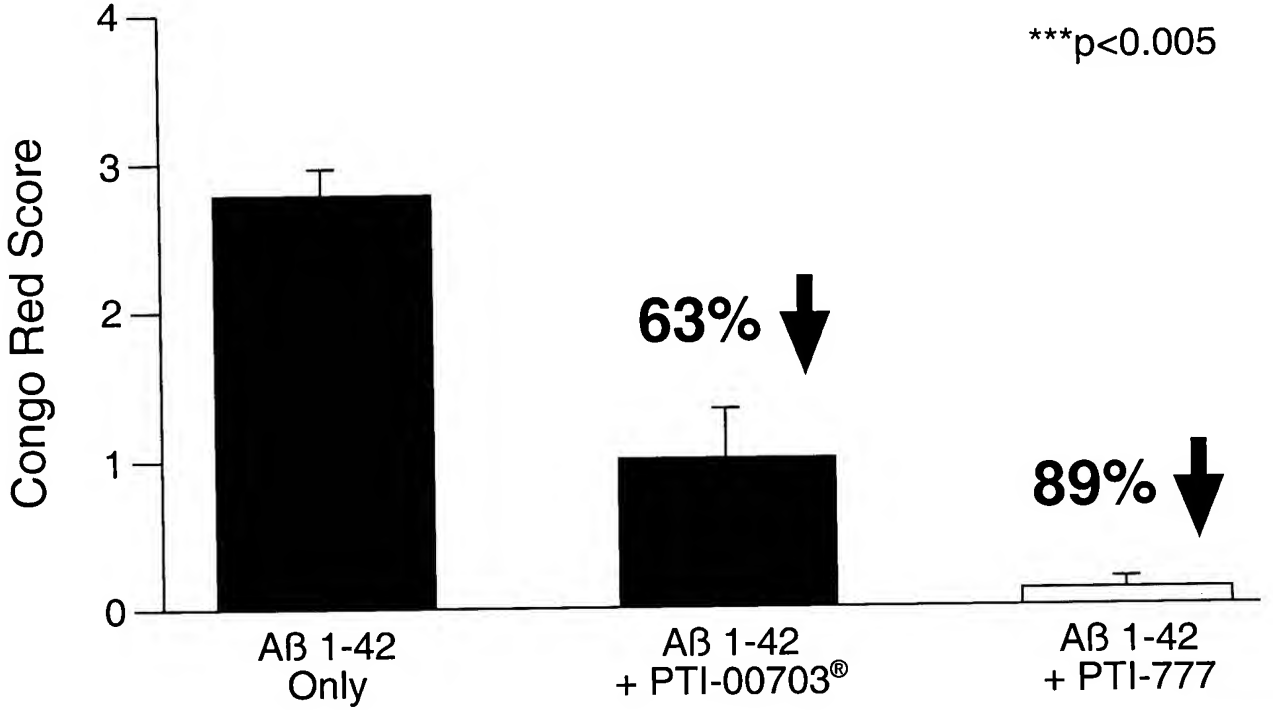
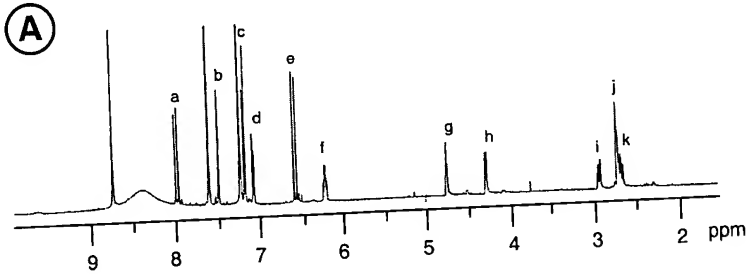


FIGURE 8

FIGURE 4



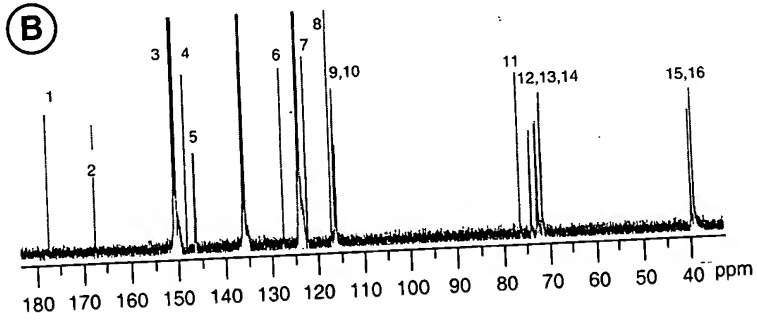
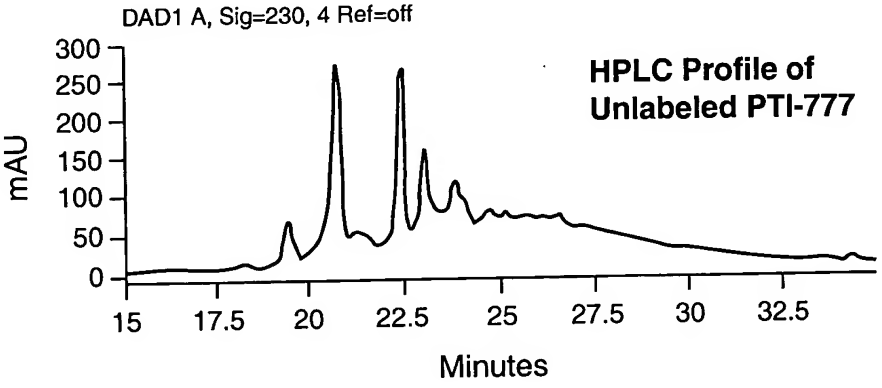
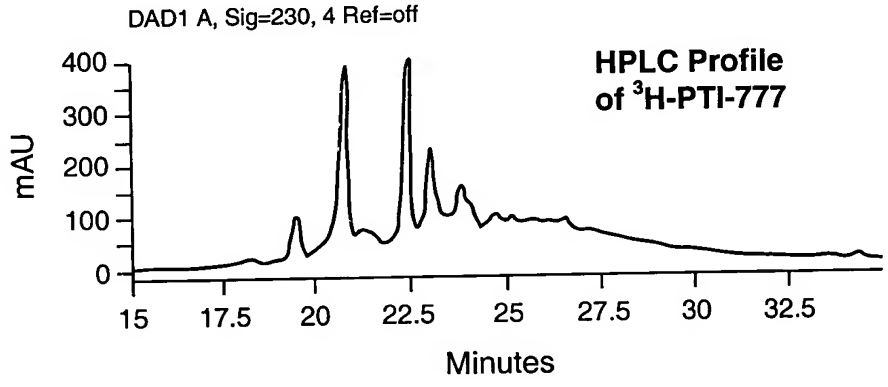


FIGURE 10

FIGURE 11





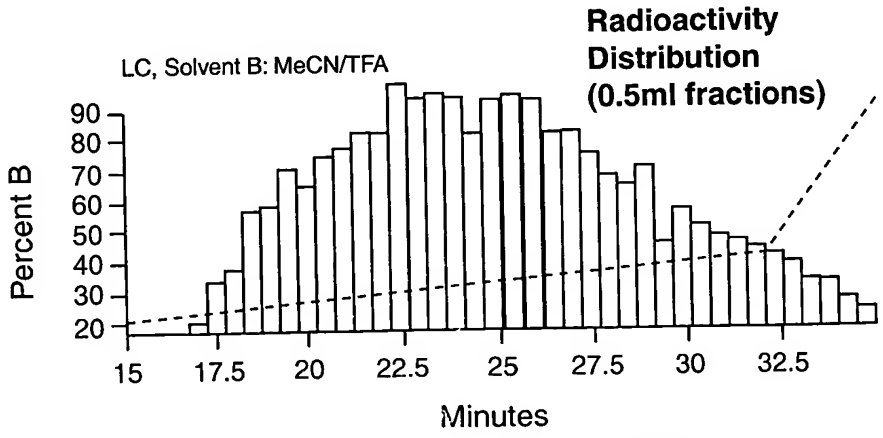


FIGURE 12

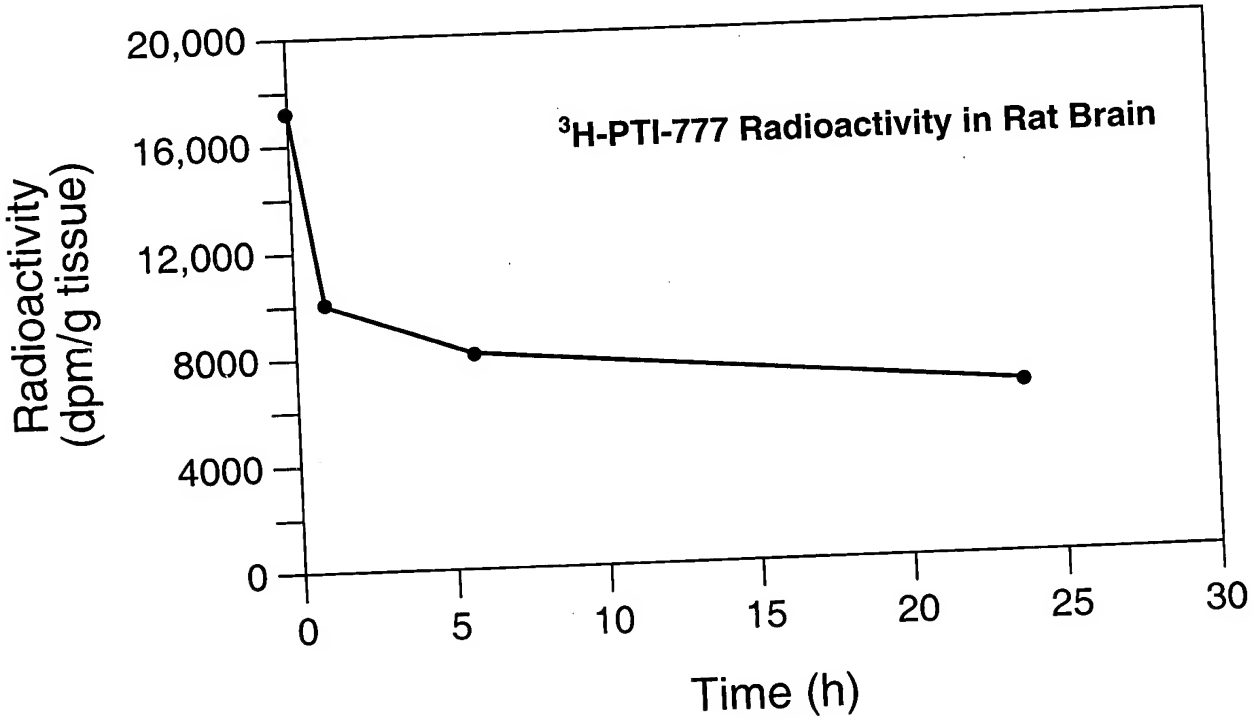


FIGURE 13

Jaguar Summed Mass Spectrum Report

File Name: G:__41.dat
Method Name:
Sample ID:
Instrument: JAGUAR

Time Run: 11/13/00 11:01:40 AM
Report Created: 11/13/00 11:03:26 AM
Operator:
Ionization Mode: ESI - positive ions

Spec # Range: 2706 - 2778

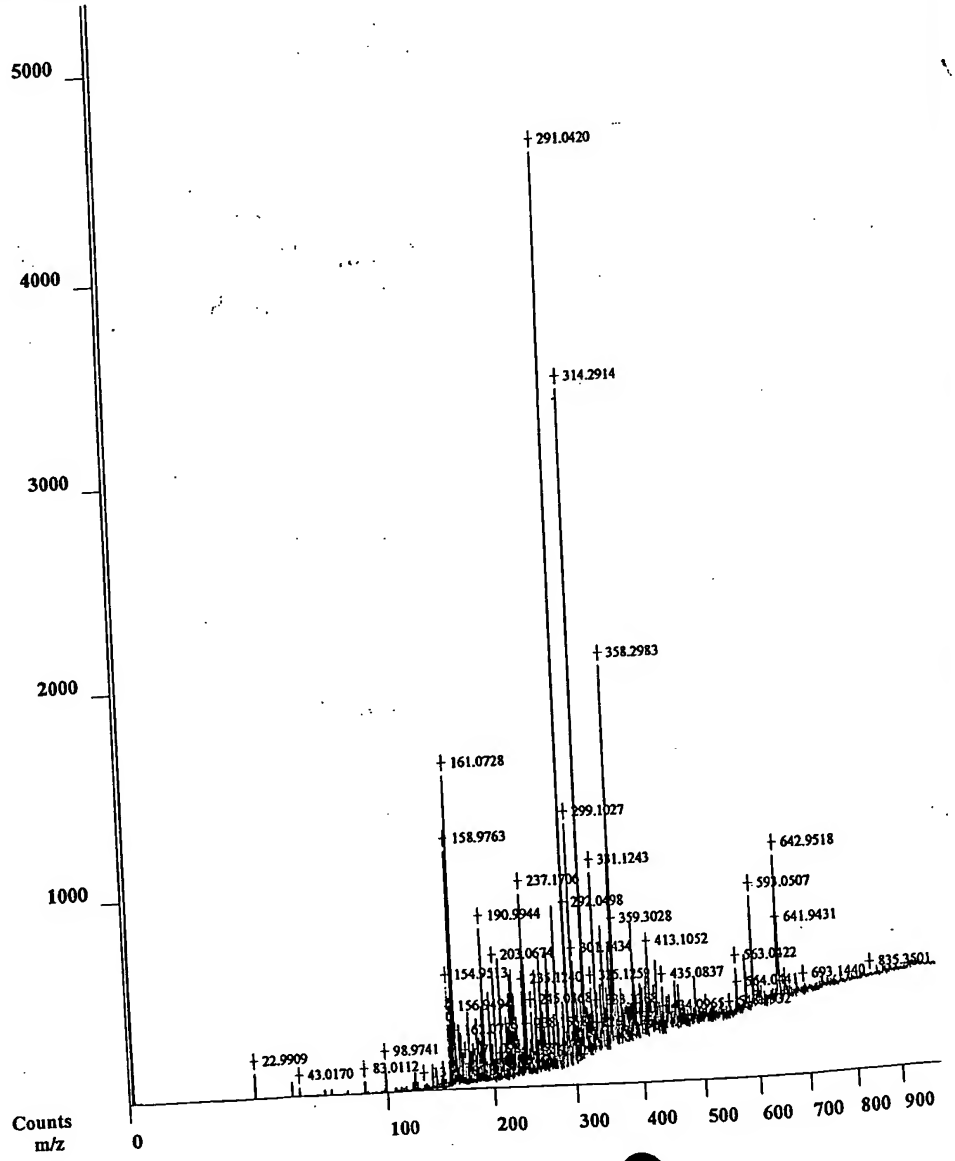


FIGURE 14

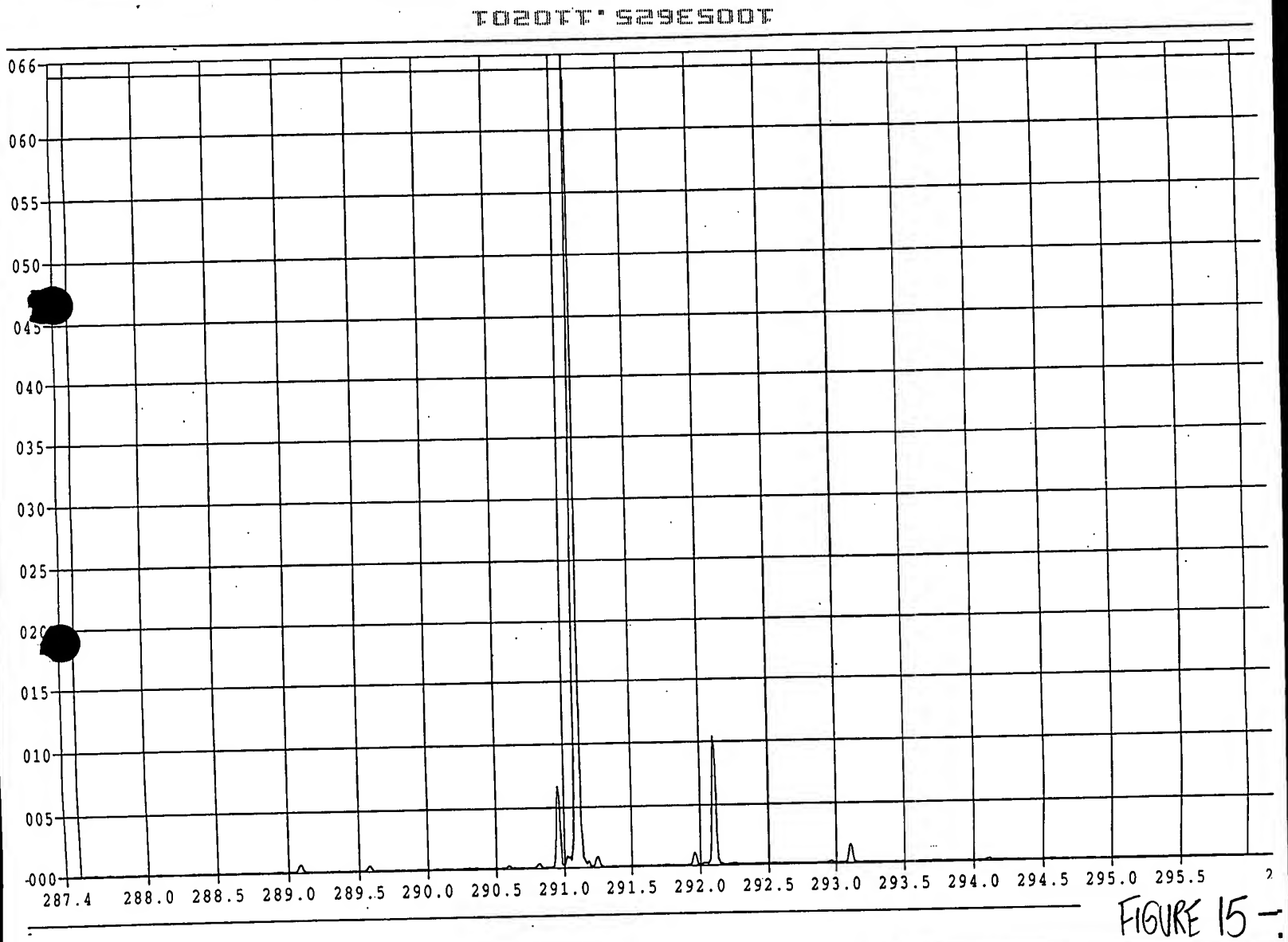
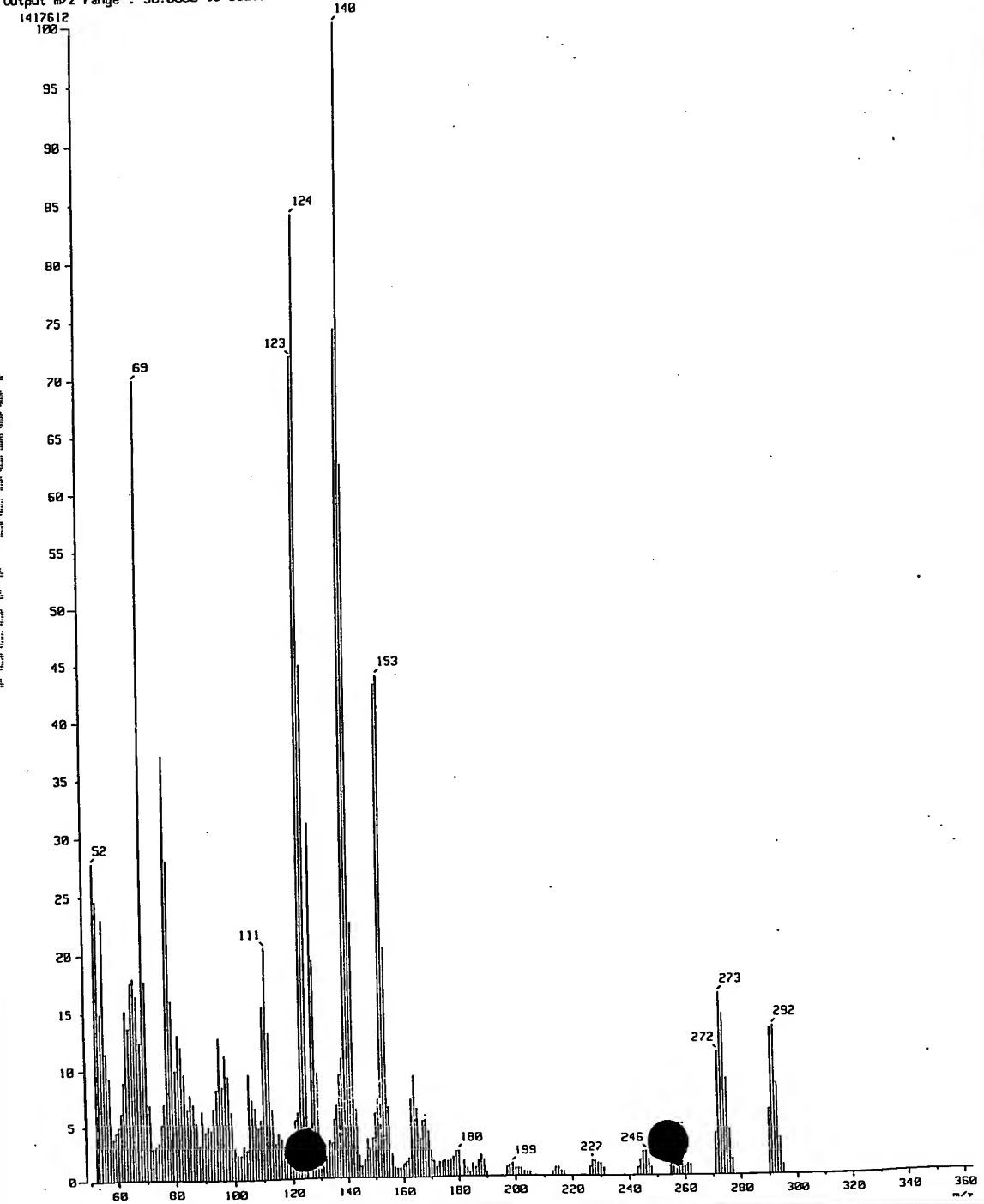

T020FF' S29E500T
066
060
055
050
045
040
035
030
025
020
015
010
005
-000
287.4
288.0
288.5
289.0
289.5
290.0
290.5
291.0
291.5
292.0
292.5
293.0
293.5
294.0
294.5
295.0
295.5

FIGURE 15 –

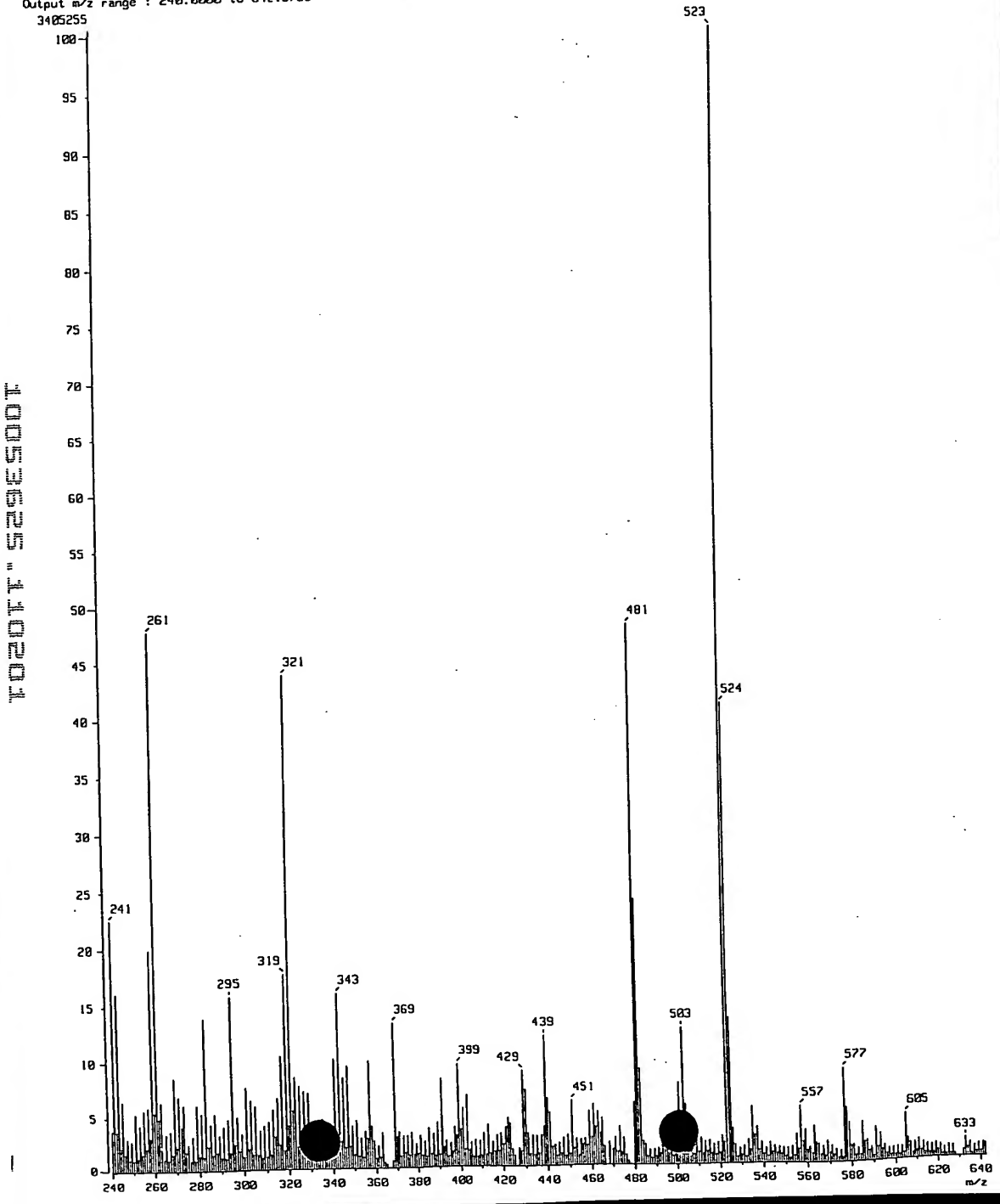
[Mass Spectrum]
Data : BYU_A776
Sample: 1
Note :
Inlet : Direct
Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.64 min
Scan# : (5,8)
BP : m/z 140.0000
Int. : 135.19
Output m/z range : 50.0000 to 362.6855
Cut Level : 0.00 %

FIGURE 16



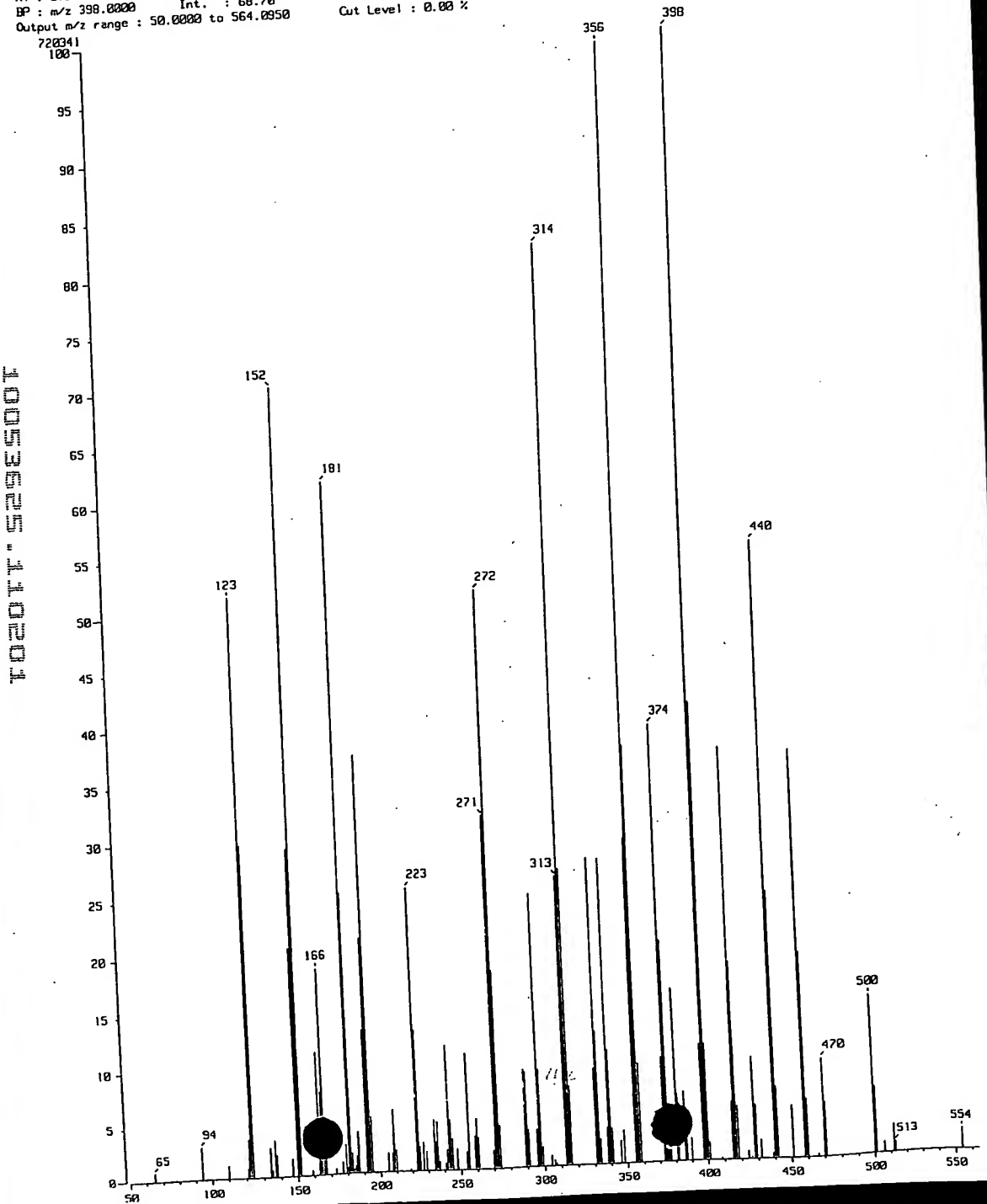
[Mass Spectrum]
Data : BYU_FB49
Sample: acylated 1
Note : ThioGlycerol & Na
Inlet : Direct
Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.08 min
Scan# : (1,4)
BP : m/z 523.0000
Int. : 322.38
Output m/z range : 240.0000 to 642.3739
Cut Level : 0.00 %

FIGURE 17



[Mass Spectrum]
Data : BYU_A373
Sample: acylated-1
Note :
Inlet : Direct
Ion Mode : EI+
Spectrum Type : Normal Ion [MF-Linear]
RT : 0.89 min
Scan# : (7,9)-k((3,4))[k=1.0]
BP : m/z 398.0000
Int. : 68.70
Output m/z range : 50.0000 to 564.0950
Cut Level : 0.00 %

FIGURE 18



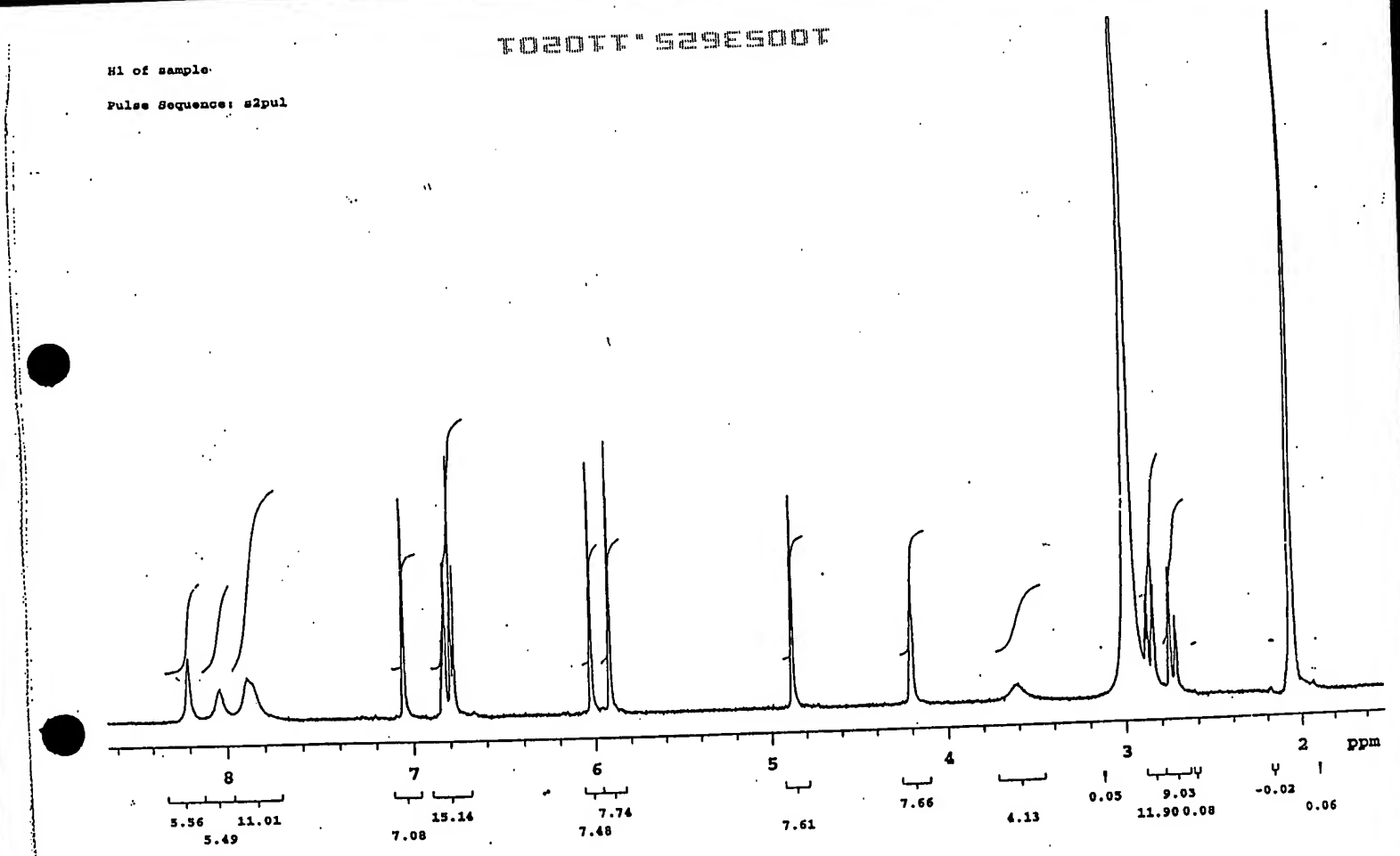

T020TT* S29ES00T
H1 of sample
Pulse Sequence: s2pul
8
7
6
5
4
3
2
ppm
5.56
11.01
5.49
7.08
15.14
7.74
7.48
7.61
7.66
4.13
0.05
9.03
11.90
0.08
-0.02
0.06

FIGURE 19

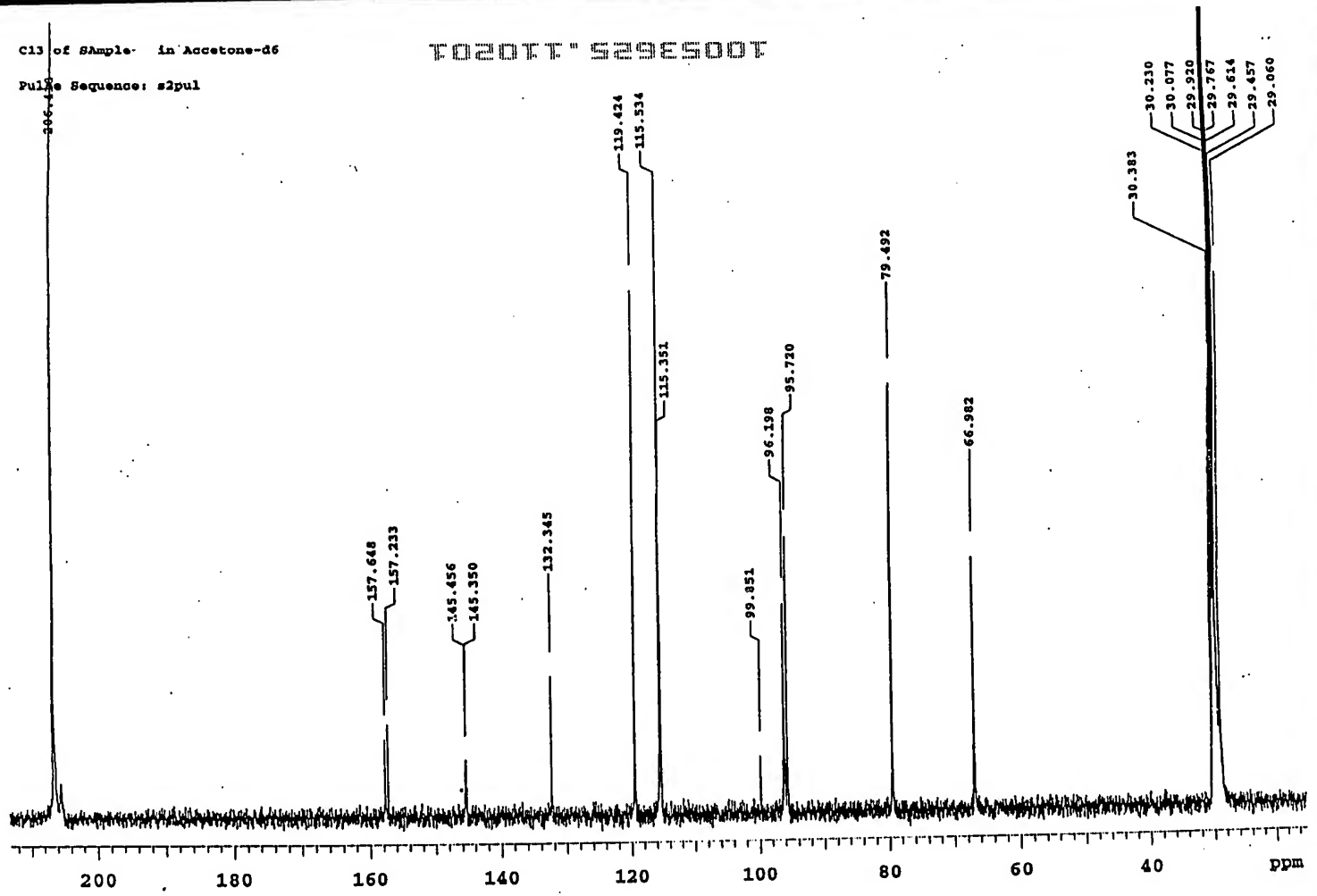

C13 of SAmple- in Accetone-d6
Pulse Sequence: s2pul
TD2DTT" 529650DT
206.418
157.648
157.233
145.456
145.350
132.345
119.424
115.534
115.351
99.851
96.198
95.720
79.492
66.982
30.383
30.230
30.077
29.920
29.767
29.614
29.457
29.060
200
180
160
140
120
100
80
60
40
ppm

FIGURE 20

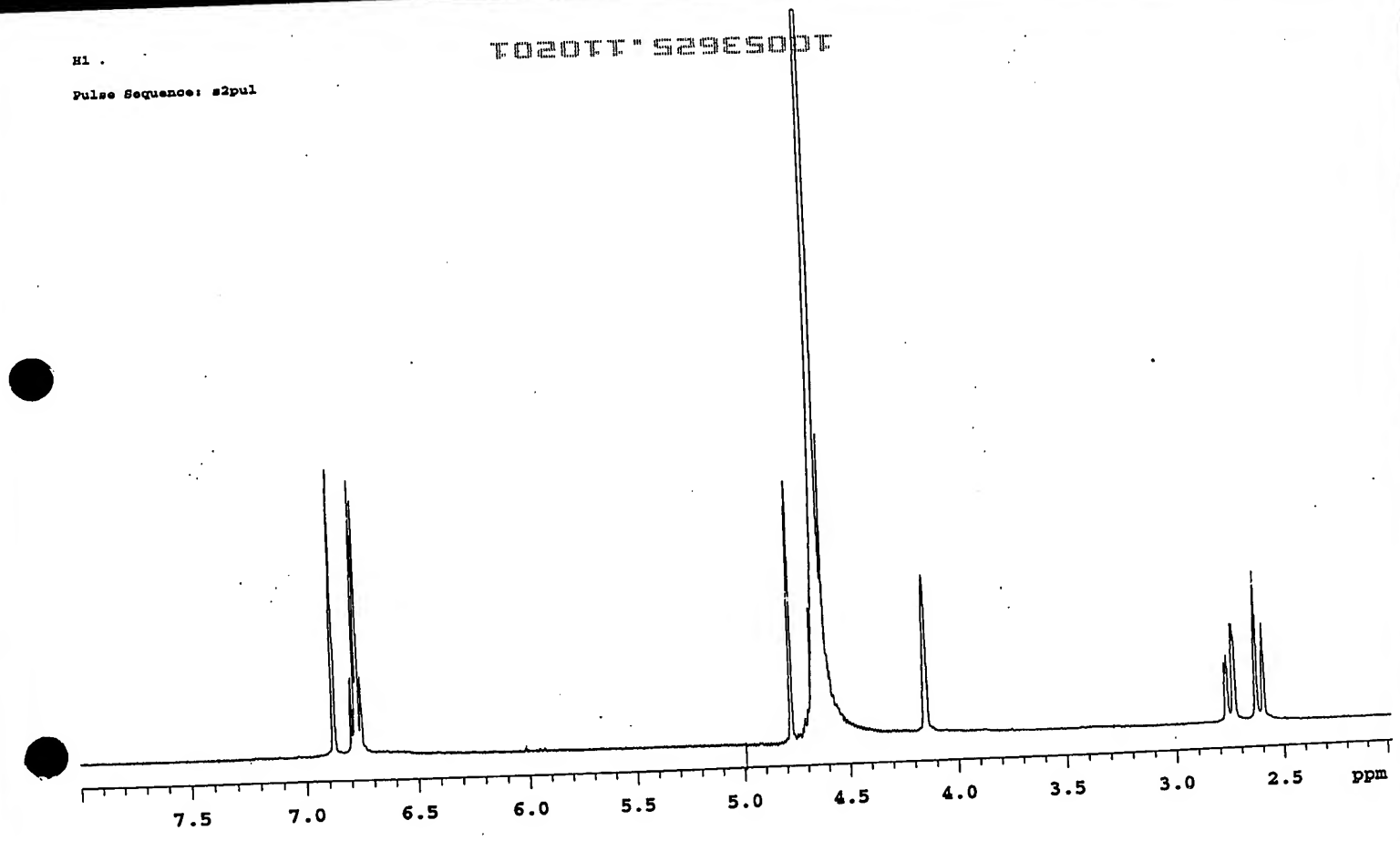


FIGURE 21

C13 of Sample in D20.

Pulse Sequence: s2pul

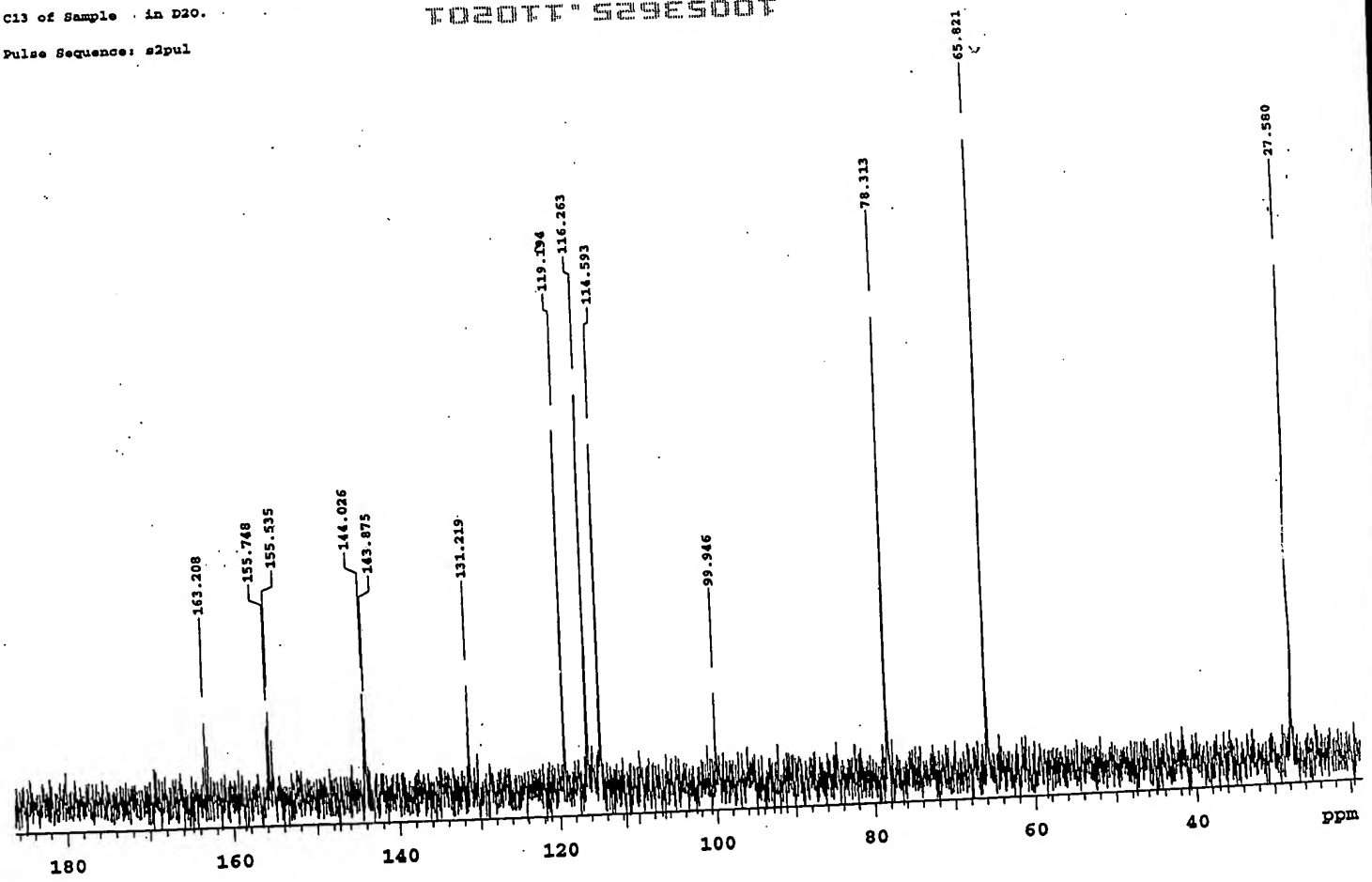


FIGURE 22

COSY of Sample

Pulse Sequence: relayh

Solvent: Acetone
Ambient temperature
UNITY-500 "nmr500"

PULSE SEQUENCE: relayh
COSY 90-90
Acq. time 0.302 sec
Width 3817.5 Hz
2D Width 3817.5 Hz
16 repetitions
159 increments
OBSERVE H1, 499.8814428 MHz
DATA PROCESSING
F1 DATA PROCESSING
Line broadening 0.3 Hz
FT size 1024 x 1024
Total time 14 min, 12 sec

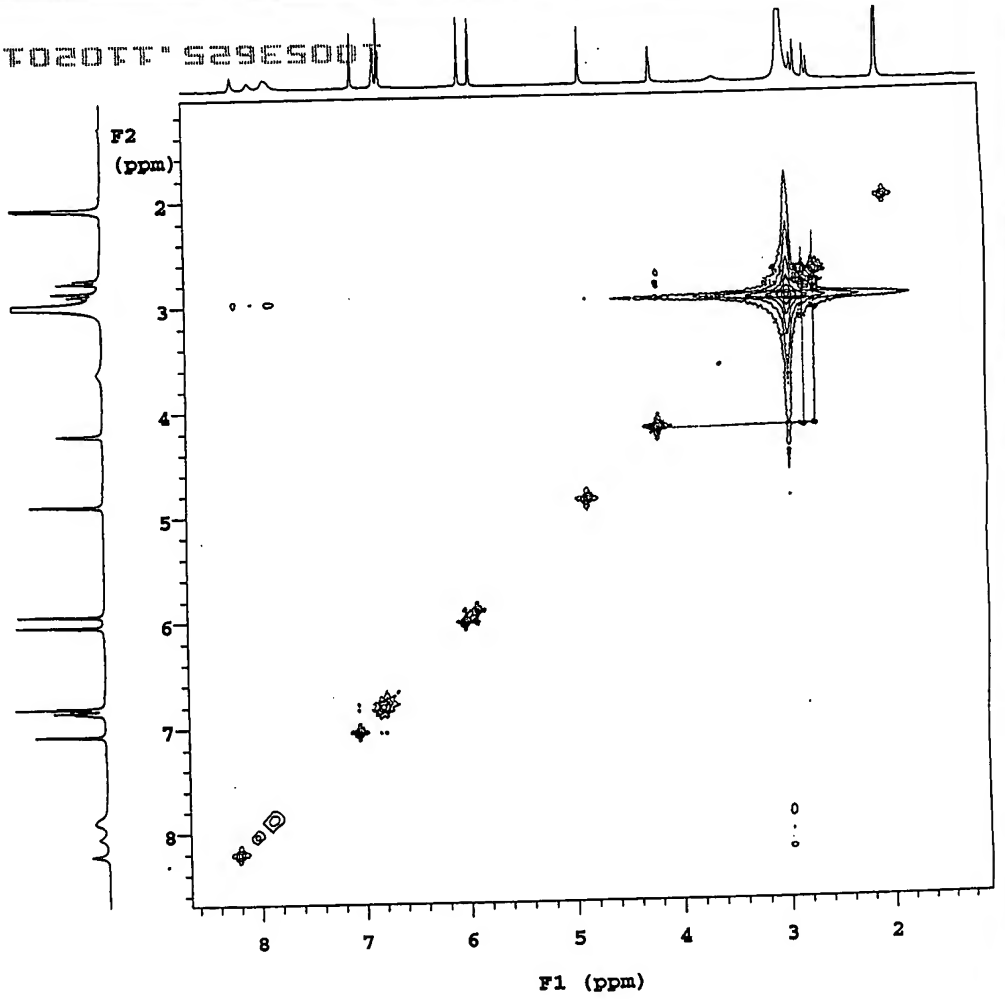


FIGURE 23

COSY

Pulse Sequence: relayh

Solvent: D2O
Ambient temperature
UNITY-500 "nmr500"

PULSE SEQUENCE: relayh
Relax. delay 0.500 sec
COSY 90-90
Acq. time 0.178 sec
Width 2882.3 Hz
2D Width 2882.3 Hz
8 repetitions
120 increments
OBSERVE H1, 499.8801324 MHz
DATA PROCESSING
Line broadening 0.1 Hz
F1 DATA PROCESSING
Line broadening 0.3 Hz
FT size 1024 x 1024
Total time 11 min, 23 sec

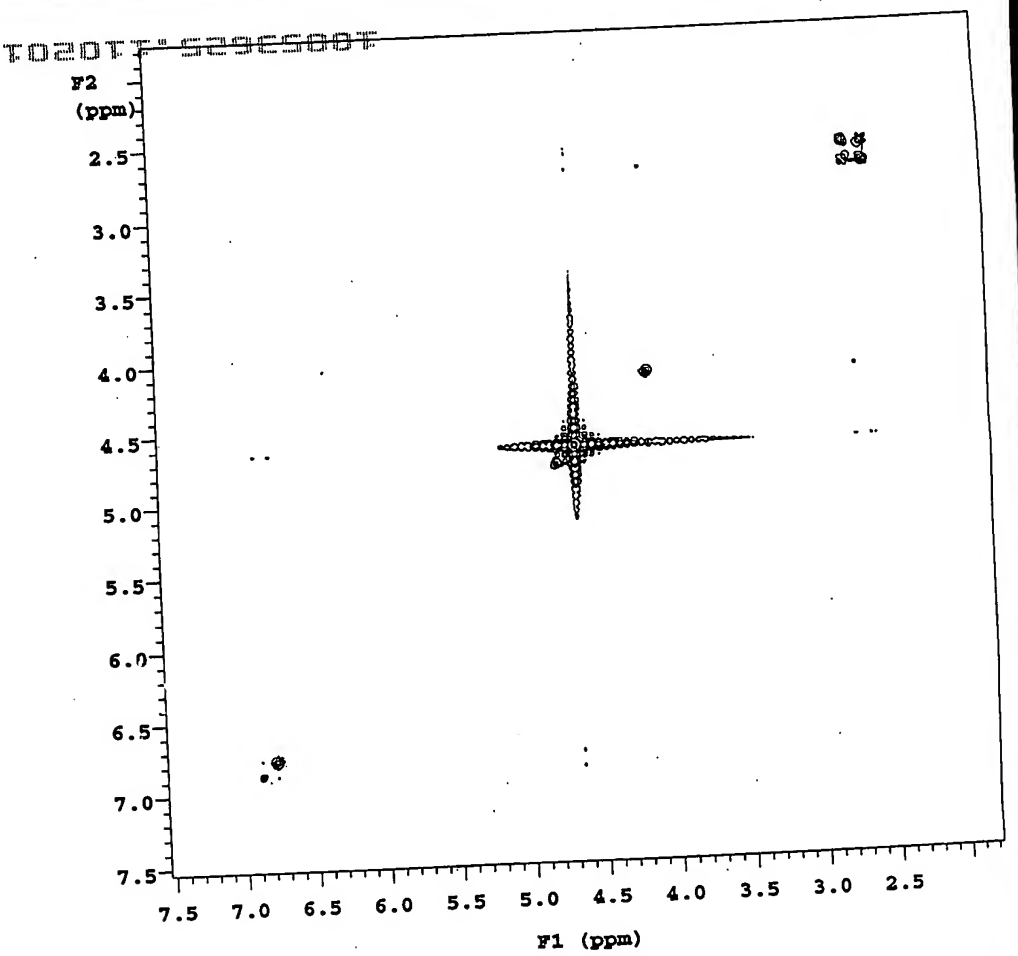


FIGURE 24A

COSY

Pulse Sequence: relayh

Solvent: D2O
Ambient temperature
UNITY-500 "nmr500"

PULSE SEQUENCE: relayh
Relax. delay 0.500 sec
COSY 90-90
Acq. time 0.178 sec
Width 2882.3 Hz
2D Width 2882.3 Hz
8 repetitions
120 increments
OBSERVE H1, 499.8801324 MHz
DATA PROCESSING
Line broadening 0.1 Hz
F1 DATA PROCESSING
Line broadening 0.3 Hz
FT size 1024 x 1024
Total time 11 min, 23 sec

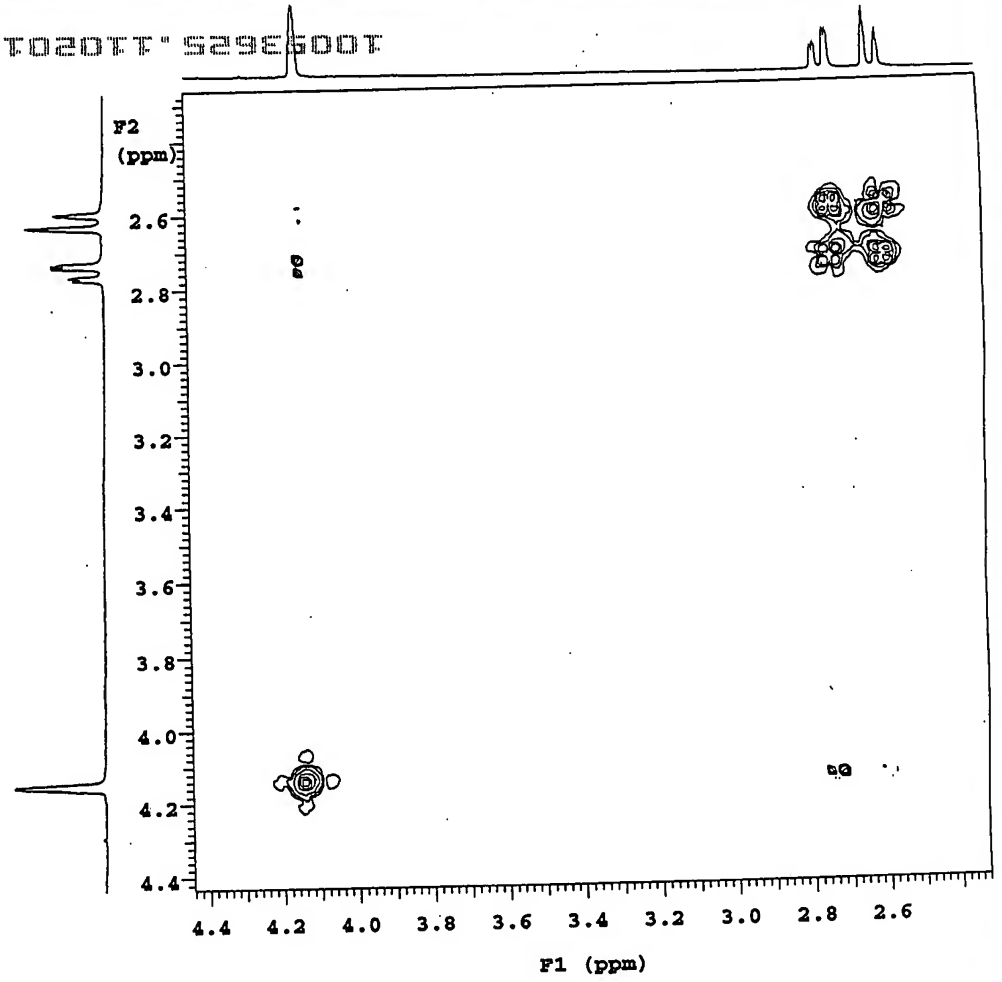


FIGURE 24B

COSY

Pulse Sequence: relayh

Solvent: D2O
Ambient temperature
UNITY-500 "nmr500"

PULSE SEQUENCE: relayh
Relax. delay 0.500 sec
COSY 90-90
Acq. time 0.178 sec
Width 2882.3 Hz
2D Width 2882.3 Hz
8 repetitions
120 increments
OBSERVE H1, 499.8801324 MHz
DATA PROCESSING
Line broadening 0.1 Hz
F1 DATA PROCESSING
Line broadening 0.3 Hz
FT size 1024 x 1024
Total time 11 min, 23 sec

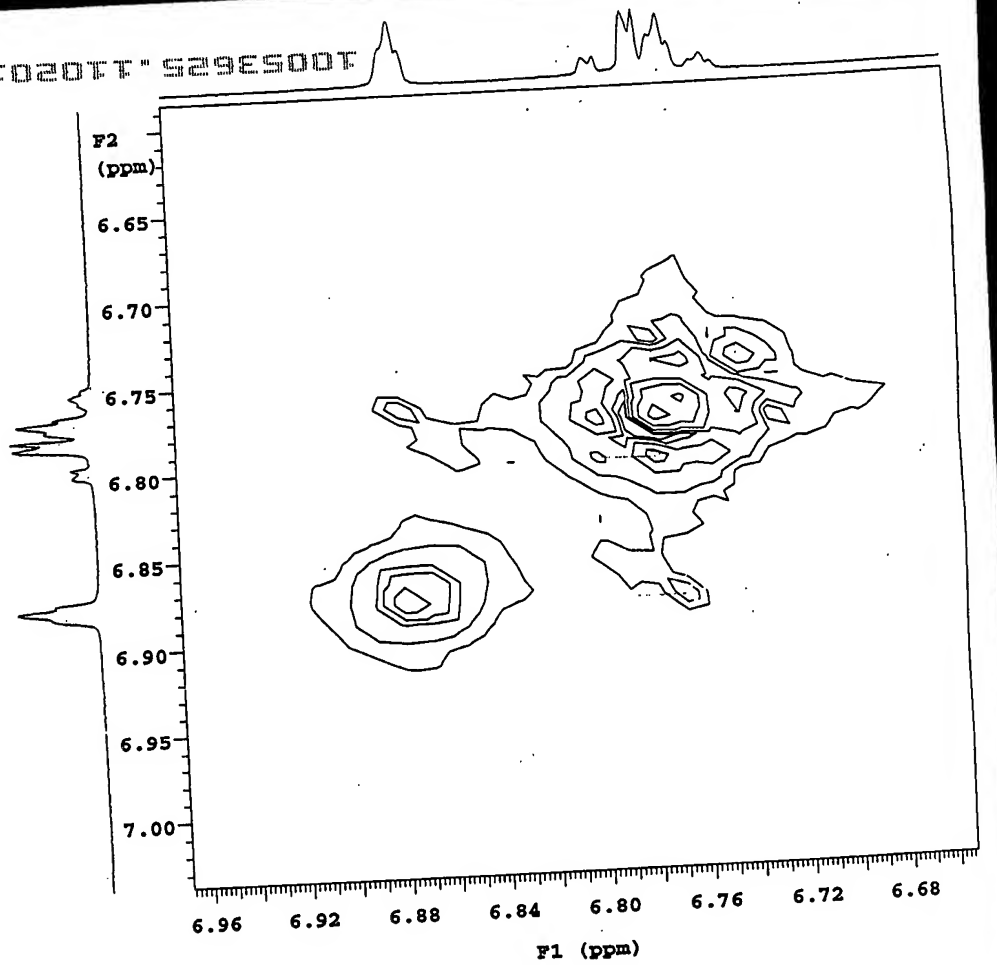


FIGURE 24C

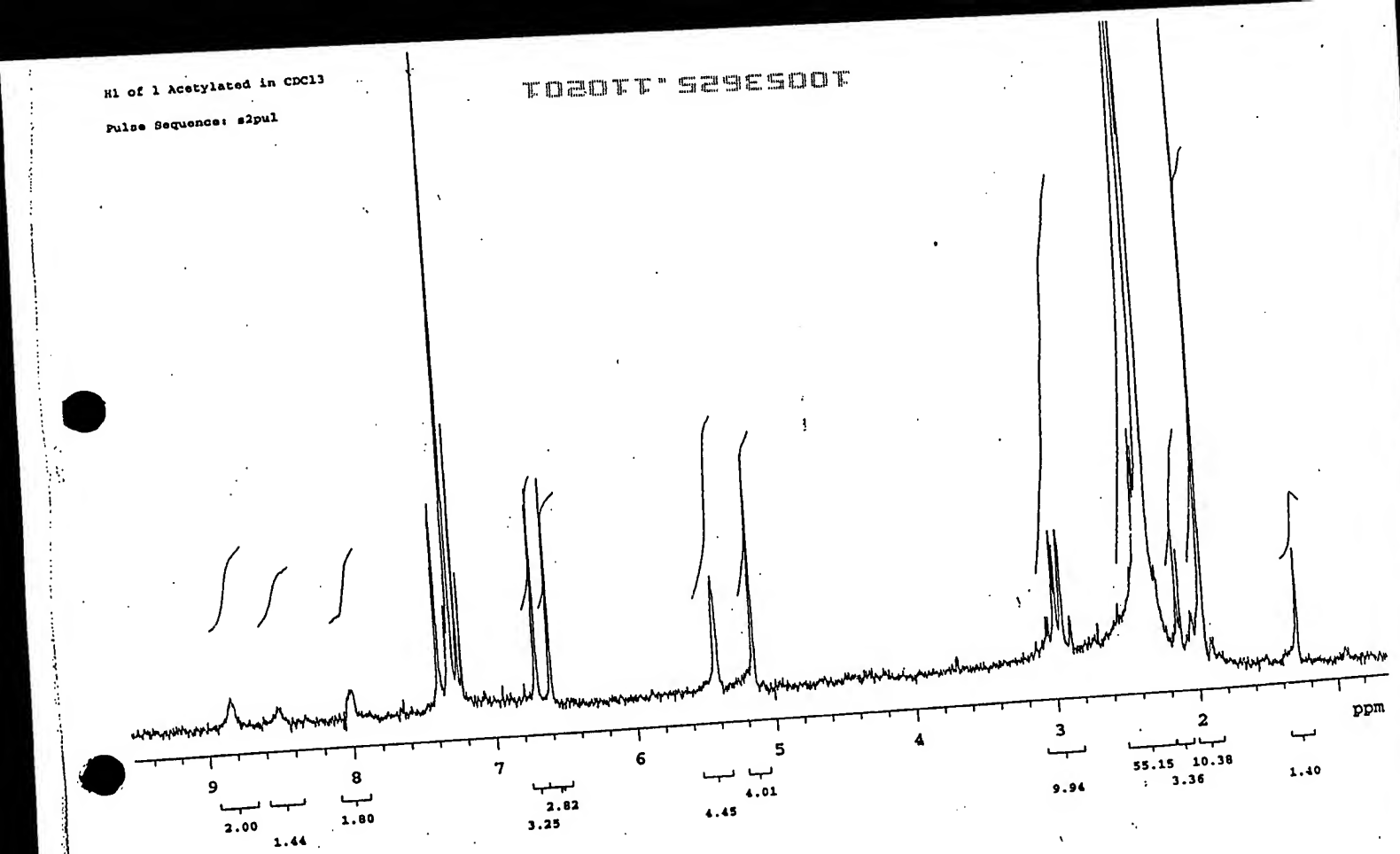
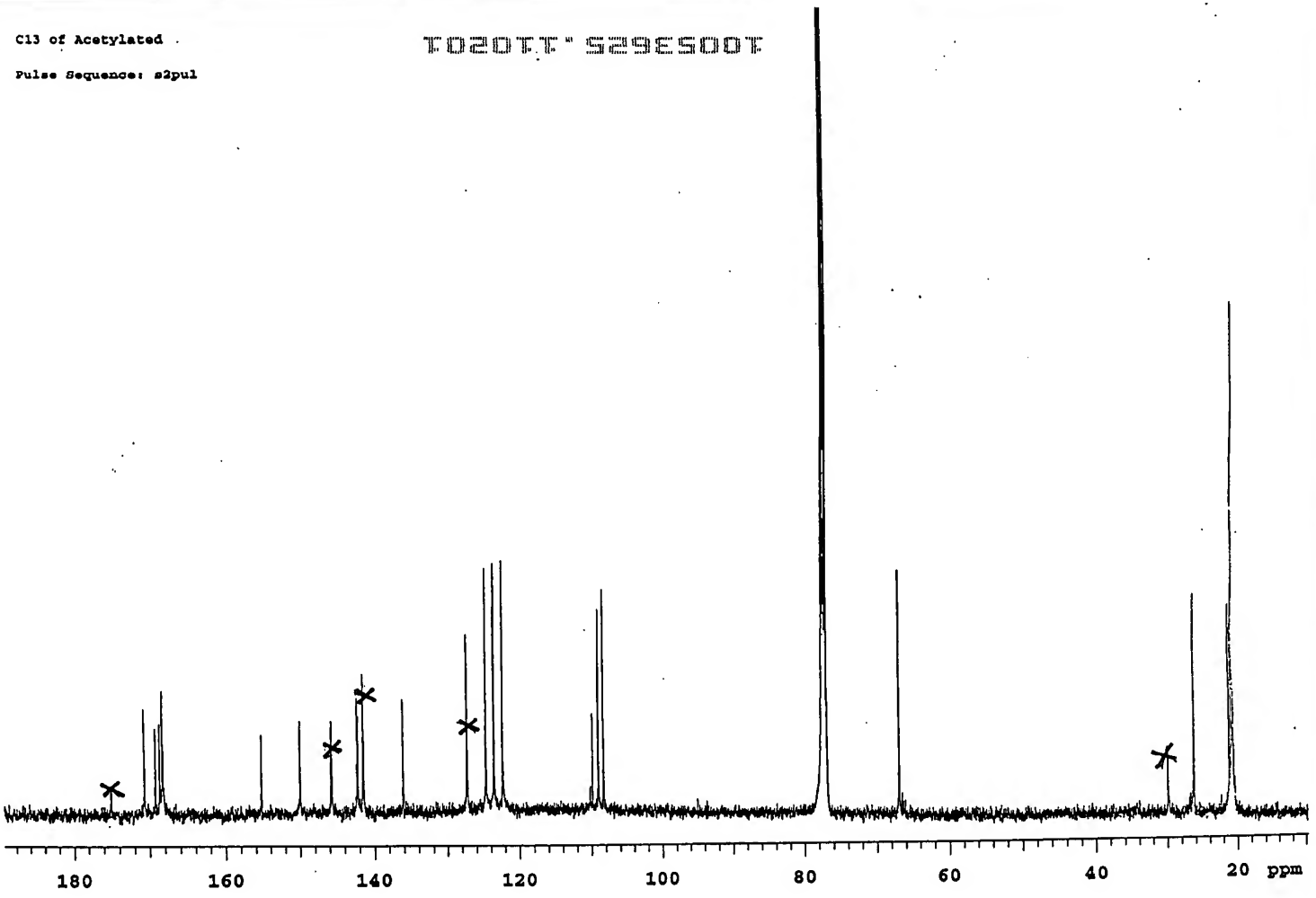

H1 of 1 Acetylated in CDCl3
Pulse Sequence: s2pul
T020TT" 529E5D0T
ppm
9
8
7
6
5
4
3
2
2.00
1.44
1.80
3.25
2.82
4.45
4.01
9.94
55.15
3.36
10.38
1.40

FIGURE 25

C13 of Acetylated

Pulse Sequence: s2pul

T020TT" S29E50DT



X= pyridinium acetate

FIGURE 26

COSY

Pulse Sequence: relayh

Solvent: CDCl3
Temp. 26.0 C / 299.1 K
INOVA-500 "nmr500"

Relax. delay 0.500 sec
COSY 90-90
Acq. time 0.128 sec
Width 8000.0 Hz
2D Width 8000.0 Hz
16 repetitions
512 increments
OBSERVE H1, 499.9135718 MHz
DATA PROCESSING
Sine bell 0.064 sec
F1 DATA PROCESSING
Sine bell 0.032 sec
FT size 2048 x 2048
Total time 1 hr, 31 min, 32 sec

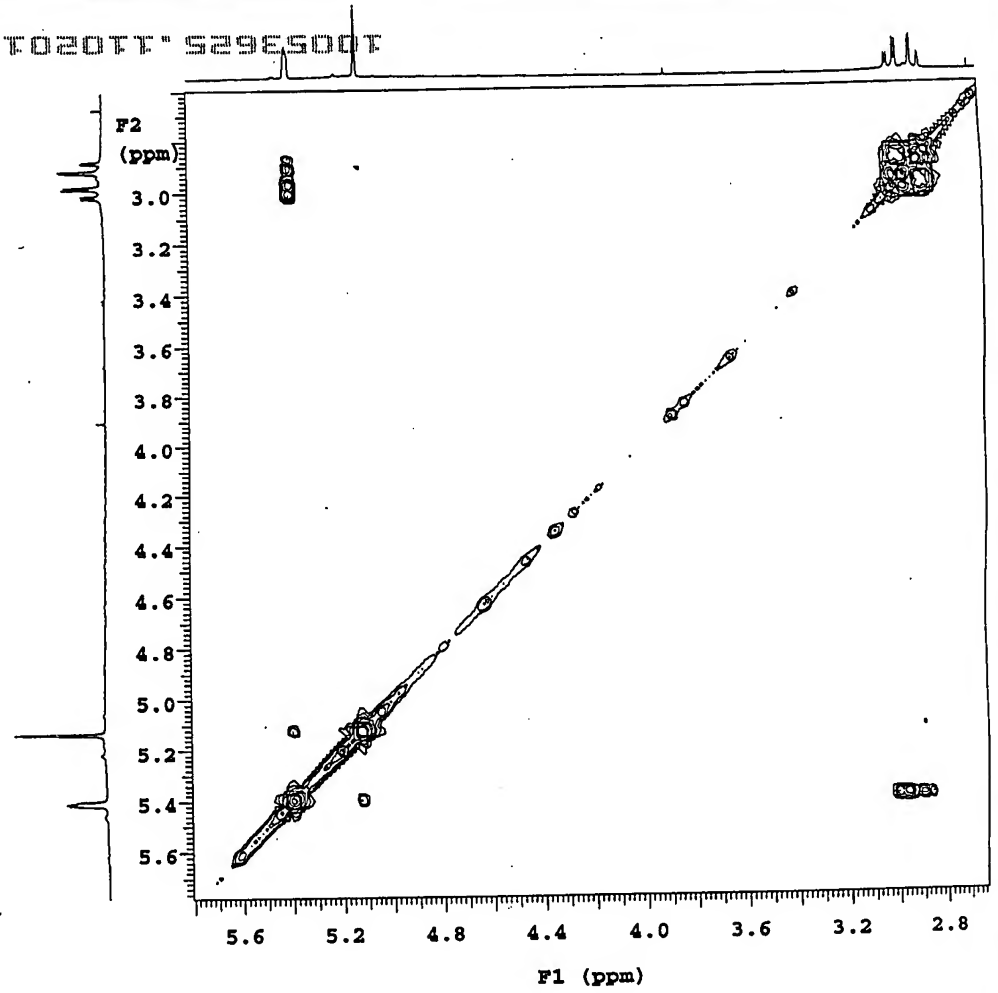


FIGURE 27

HETCOR of Acetylated . in CDCl3.

Pulse Sequence: hetcor

Solvent: CDCl3
Temp. 26.0 C / 299.1 K
User: 1-14-87
INOVA-500 "nmr500"

Relax. delay 1.000 sec
Acq. time 0.082 sec
Width 25000.0 Hz
2D Width 4614.9 Hz
208 repetitions
256 increments
OBSERVE C13, 125.7033376 MHz
DECOUPLE H1, 499.9160715 MHz
Power 38 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
F1 DATA PROCESSING
Line broadening 0.3 Hz
FT size 4096 x 1024
Total time 16 hr, 46 min, 21 sec

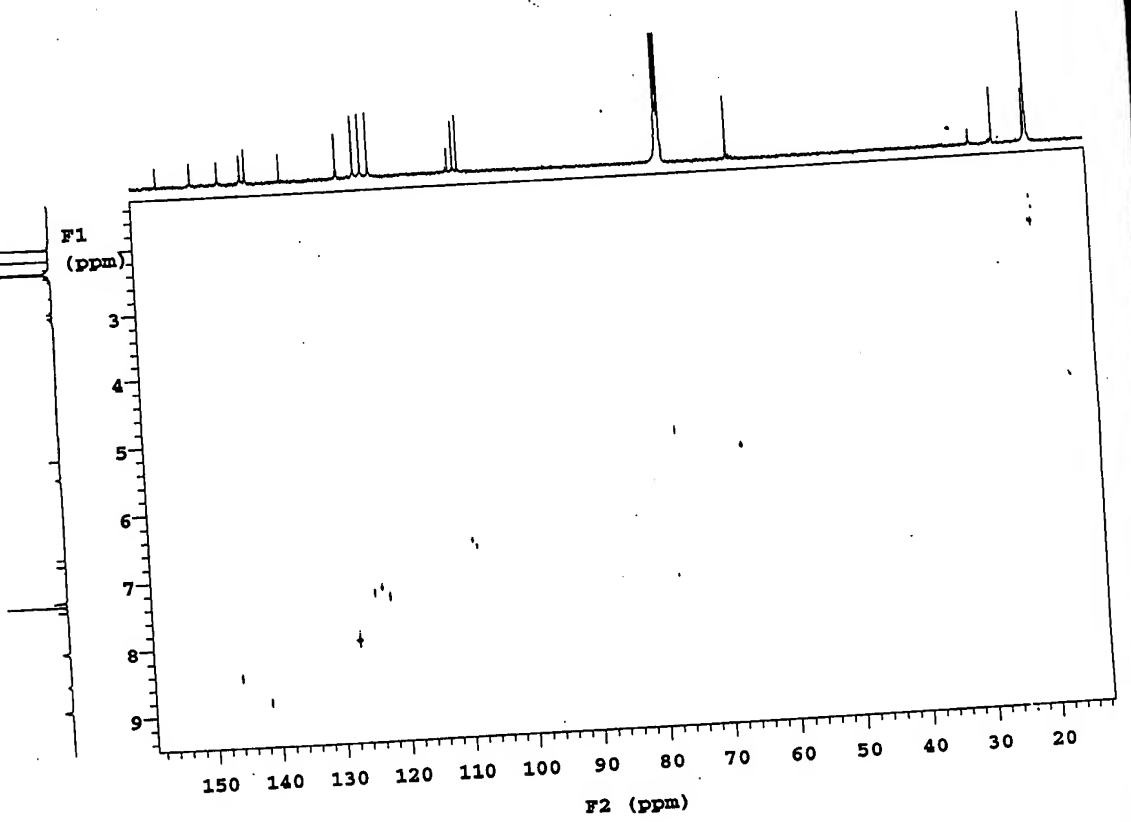


FIGURE 28A

HETCOR of Acetylated · in CDCl3.

Pulse Sequence: hetcor

Solvent: CDCl3
Temp. 26.0 C / 299.1 K
User: 1-14-87
INOVA-500 "nmr500"

Relax. delay 1.000 sec
Acq. time 0.082 sec
Width 25000.0 Hz
2D Width 4614.9 Hz
208 repetitions
256 increments
OBSERVE C13, 125.7033376 MHz
DECOUPLE H1, 499.9160715 MHz
Power 38 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
F1 DATA PROCESSING
Line broadening 0.3 Hz
FT size 4096 x 1024
Total time 16 hr, 46 min, 21 sec

TO2OTF "6295 6207

X = pyridinium acetate

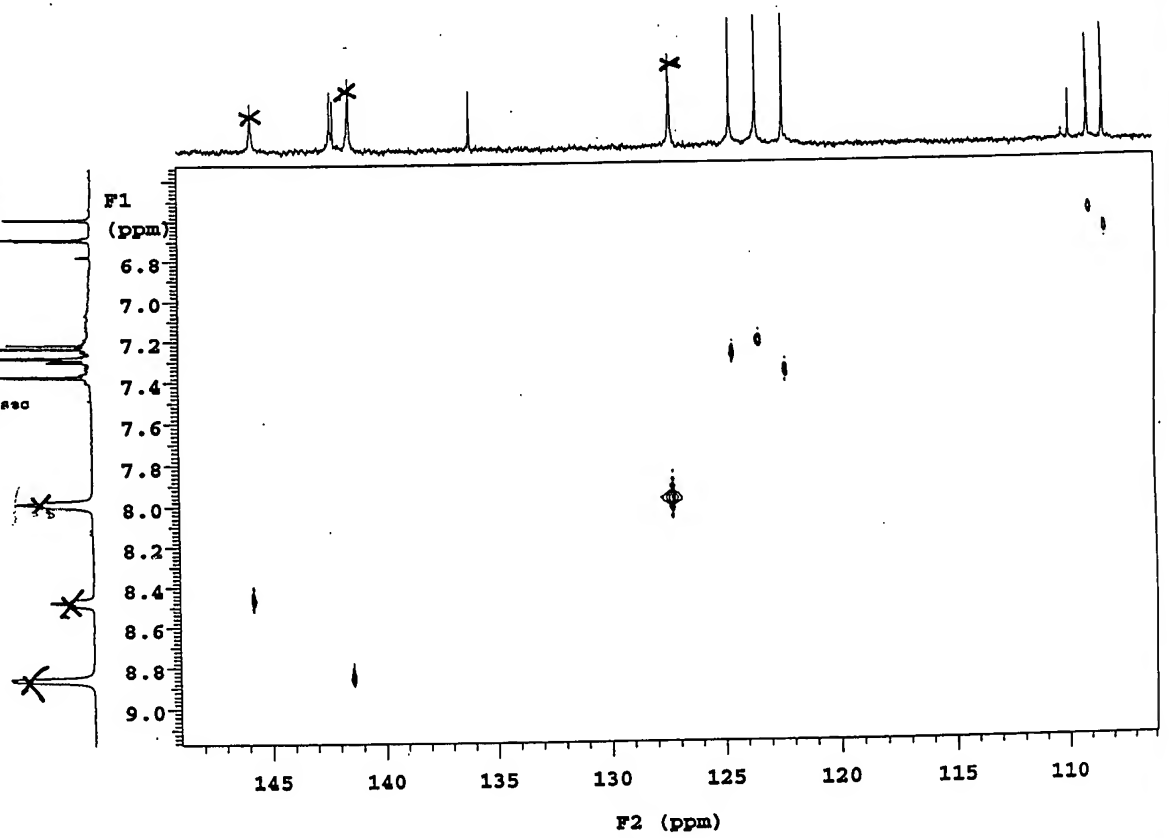


FIGURE 28B

HETCOR of Acetylated . in CDCl3.

Pulse Sequence: hetcor

Solvent: CDCl3
Temp. 26.0 C / 299.1 K
User: 1-14-87
INOVA-500 "nmr500"

Relax. delay 1.000 sec
Acq. time 0.082 sec
Width 25000.0 Hz
2D Width 4614.9 Hz
208 repetitions
256 increments
OBSERVE C13, 125.7033376 MHz
DECOUPLE H1, 499.9160715 MHz
Power 38 dB
on during acquisition
off during delay
WALTZ-16 modulated
DATA PROCESSING
Line broadening 2.0 Hz
F1 DATA PROCESSING
Line broadening 0.3 Hz
FT size 4096 x 1024
Total time 16 hr, 46 min, 21 secs

T020TT" 5296500T

X = pyridinium acetate

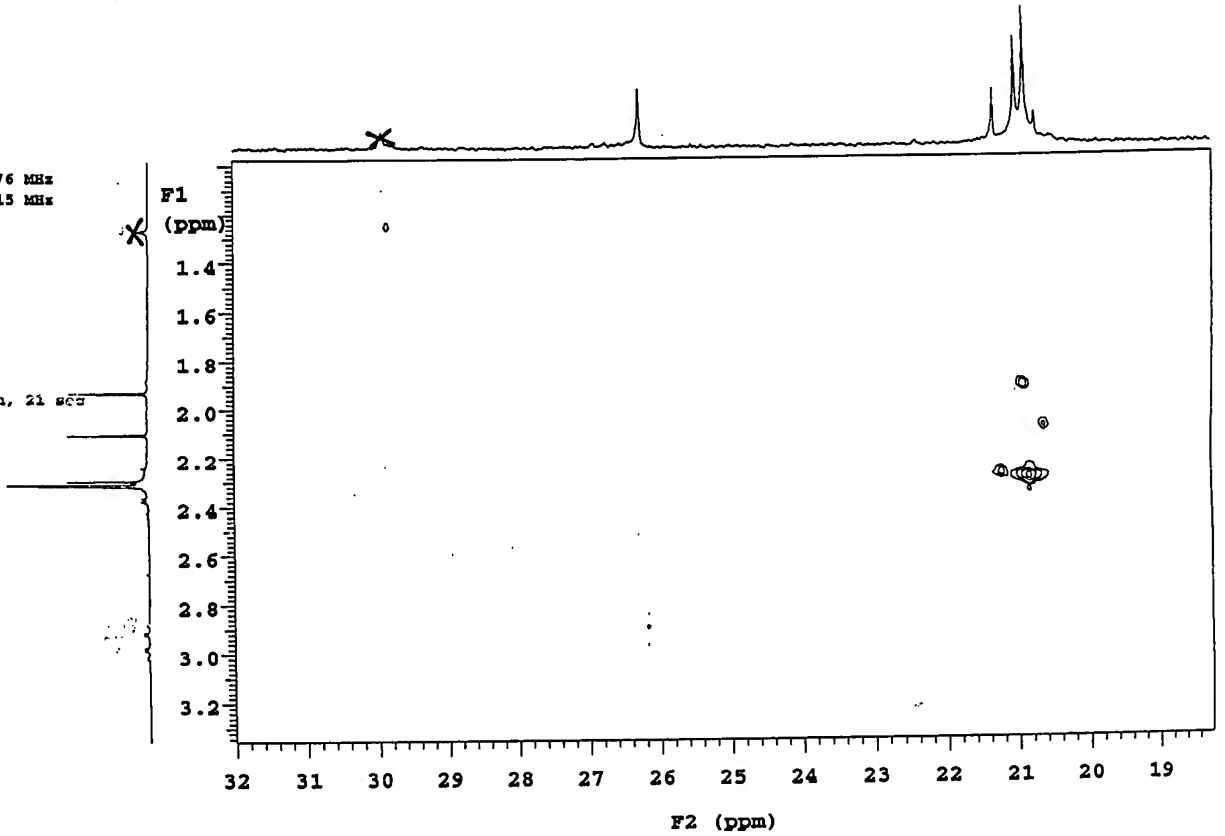


FIGURE 28C

HELP

Wavelength Scan
ReadSamples Tabulate +-*/Scans Scatter NetA Method SaveClear Print Quit

Scan directory: VIEW
Start wl: 200 nm
End wl: 400 nm
Overlay scans: [No]

Autoprint: [No]
Autosave: [No]
Scans per sample: 1
Interval: 15.00 [sec]

Method name: A:\DEFAULT
Autosave name: [A:\]SCANS
Sampling device: None
Scan speed: 600 nm/min

A:\WORK_005 (600)

Zoom ZoomOut Trace Function Autoscale Annotate Print

Functions: Scan

Smoothing: None

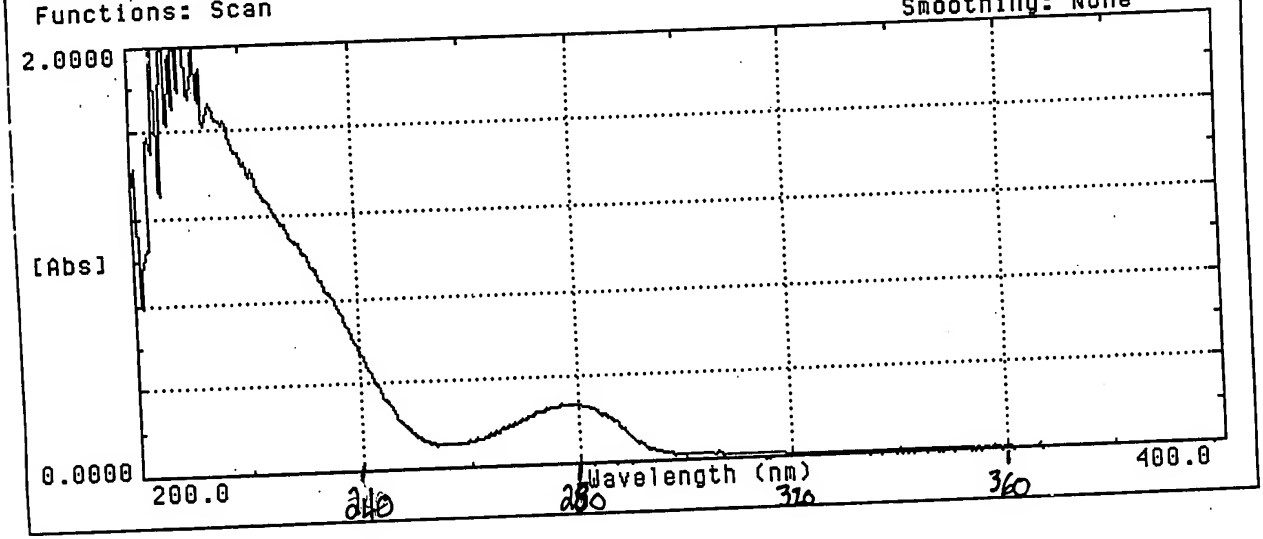


FIGURE 29

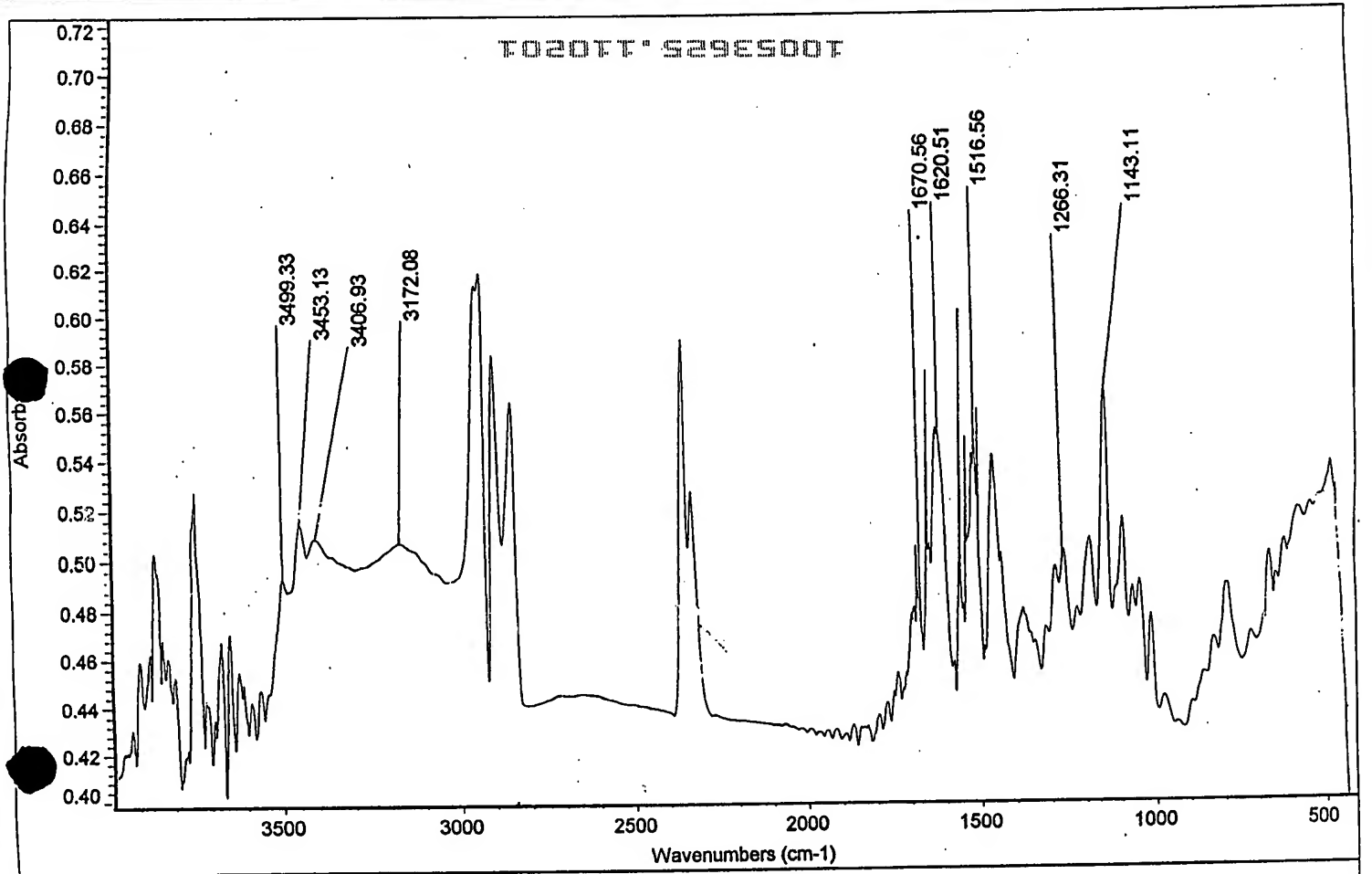

0.72
0.70
0.68
0.66
0.64
0.62
0.60
0.58
0.56
0.54
0.52
0.50
0.48
0.46
0.44
0.42
0.40
Absorb
3499.33
3453.13
3406.93
3172.08
1670.56
1620.51
1516.56
1266.31
1143.11
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)
**Subtraction Result:proteotech, sampleL
Scans: 32
Resolution: 4.000

FIGURE 30

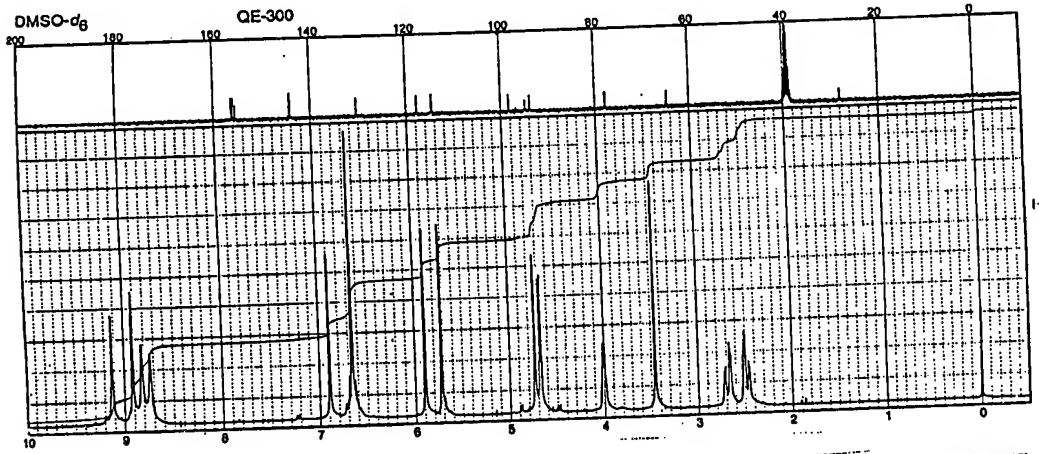
Aromatic Alcohols and Phenols

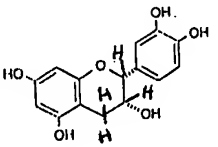
Aldrich 85,523-5 CAS [490-46-0] $C_{15}H_{14}O_6$ FW 290.27 mp 240°C d.

(-)-Epicatechin, 97%

156.31	130.42	94.89°
156.01	117.78°	93.91°
155.57	114.69°	77.88°
144.28	114.58°	64.75°
144.23	98.31	28.07

A



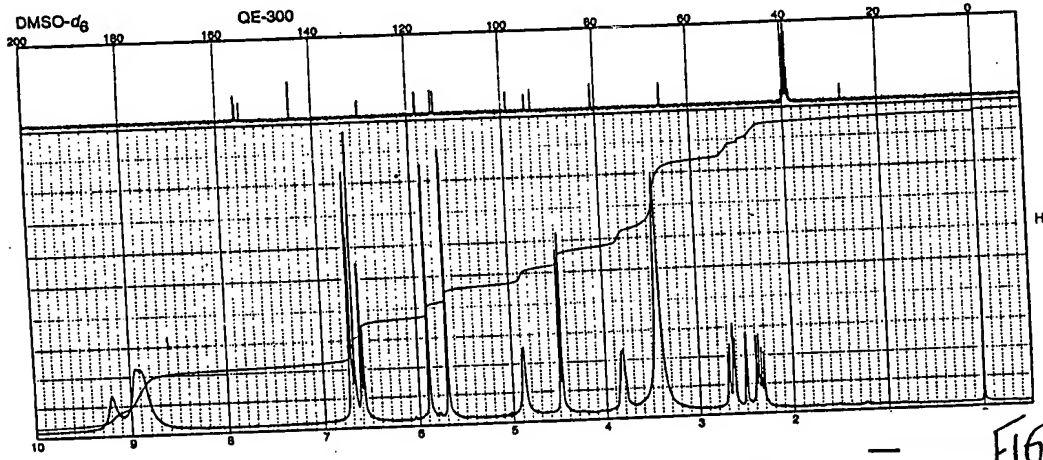


Aldrich 86,181-2 $C_{15}H_{14}O_6$ FW 290.28 mp 210°C d.

(±)-Catechin hydrate, 98%

156.25	114.35°	
155.97	98.90	
155.15	94.97°	
144.65	93.70°	
130.43	80.83°	
118.24°	66.17°	
114.92°	27.70	

C



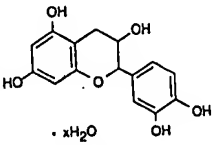


FIGURE 31

T020TT" 529E50DT

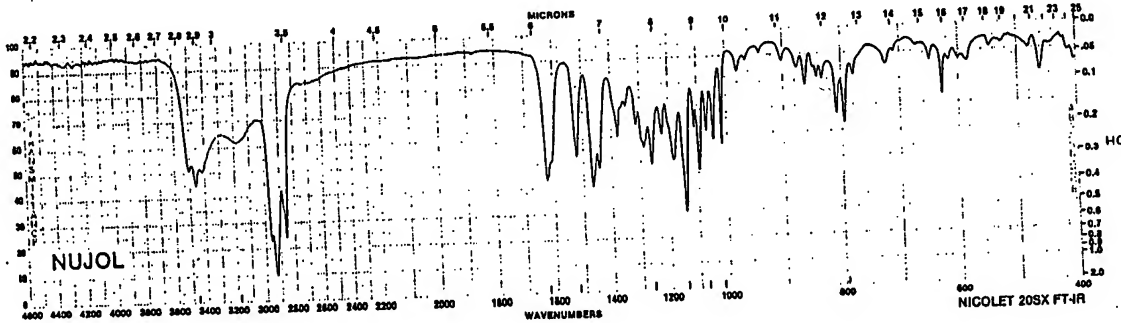
85523-5 *CAS [490-46-0]*
/-Epicatechin

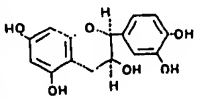
FW 290.27
mp 240°C (dec.)

IR III, 673E

3455.2 1521.4 1069.5
3176.0 1261.0 1016.8
1626.3 1144.3 794.7

D





22402-2 *CAS [154-23-4]*
(+)-Catechin hydrate

FW 290.28

IR III, 703G
Merck 10,1883

3411.2 1514.7 1144.3
3134.9 1293.2 1020.6
1609.9 1236.4 832.3

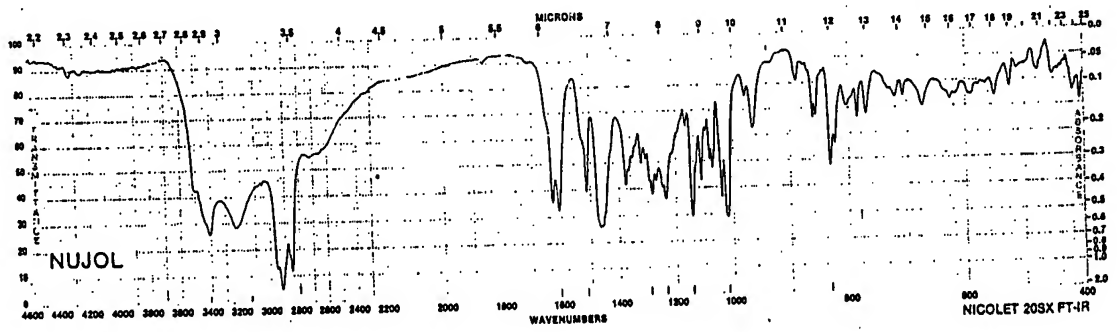


FIGURE 32

FIGURE 33

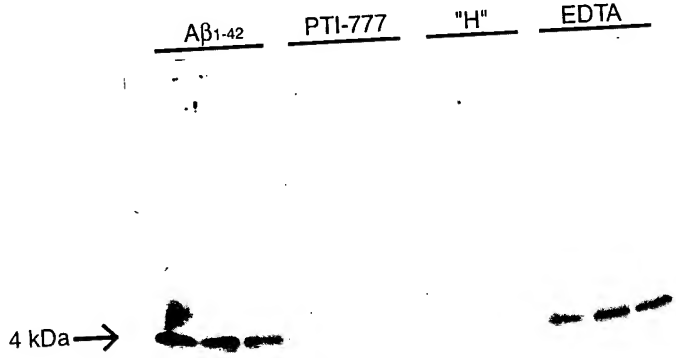


FIGURE 34